403 Poyntz Avenue, Suite B
Manhattan, KS 66502-6081
+1.785.770.8511
www.thunderheadeng.com

PetraSim User Manual

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PetraSim User Manual

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Disclaimer

Thunderhead Engineering makes no warranty, expressed or implied, to users of PetraSim, and accepts no responsibility for its use. Users of PetraSim assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that PetraSim is intended for use only by those competent in the field of multi-phase, multi-component fluid flow in porous and fractured media. PetraSim is intended only to supplement the informed judgment of the qualified user. The software package is a computer model that may or may not have predictive capability when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions. All results should be evaluated by an informed user.

Throughout this document, the mention of computer hardware or commercial software does not constitute endorsement by Thunderhead Engineering, nor does it indicate that the products are necessarily those best suited for the intended purpose.

Acknowledgements

We thank Karsten Pruess, Tianfu Xu, George Moridis, Michael Kowalsky, Curt Oldenburg, and Stefan Finsterle in the Earth Sciences Division of Lawrence Berkeley National Laboratory for their gracious responses to our many questions. We also thank Ron Falta at Clemson University and Alfredo Battistelli at Aquater S.p.A., Italy, for their help with T2VOC and TMVOC. Without TOUGH2, T2VOC, TOUGHREACT, and TOUGH-Fx/HYDRATE, PetraSim would not exist.

In preparing this manual, we have liberally used descriptions from the user manuals for the TOUGH family of codes. Links to download the TOUGH manuals are given at http://www.petrasim.com. More information about the TOUGH family of codes can be found at: http://www-esd.lbl.gov/TOUGH2/. Printed copies of the user manuals may be obtained from Karsten Pruess at <K_Pruess@lbl.gov>.

The original development of PetraSim was funded by a Small Business Innovative Research grant from the U.S. Department of Energy. Additional funding was provided by a private consortium for the TOUGHREACT version and by the U.S. Department of Energy NETL for the TOUGH-Fx/HYDRATE version.

We most sincerely thank our users for their feedback and support.

Chapter 1. Getting Started

Welcome

PetraSim is an interactive pre-processor and post-processor for the TOUGH family of codes. It helps users rapidly develop models and view results for these general purpose simulators which model nonisothermal flows of multicomponent, multiphase fluids in porous and fractured media. The T2VOC and TMVOC simulators include three-phase flows of water, air, and volatile organic chemicals. The TOUGHREACT simulator adds chemical reactions. The TOUGH-Fx/HYDRATE simulator includes the capability to represent methane hydrates.

PetraSim at a Glance

Main Window

The main window guides the user through the process of specifying all model input.

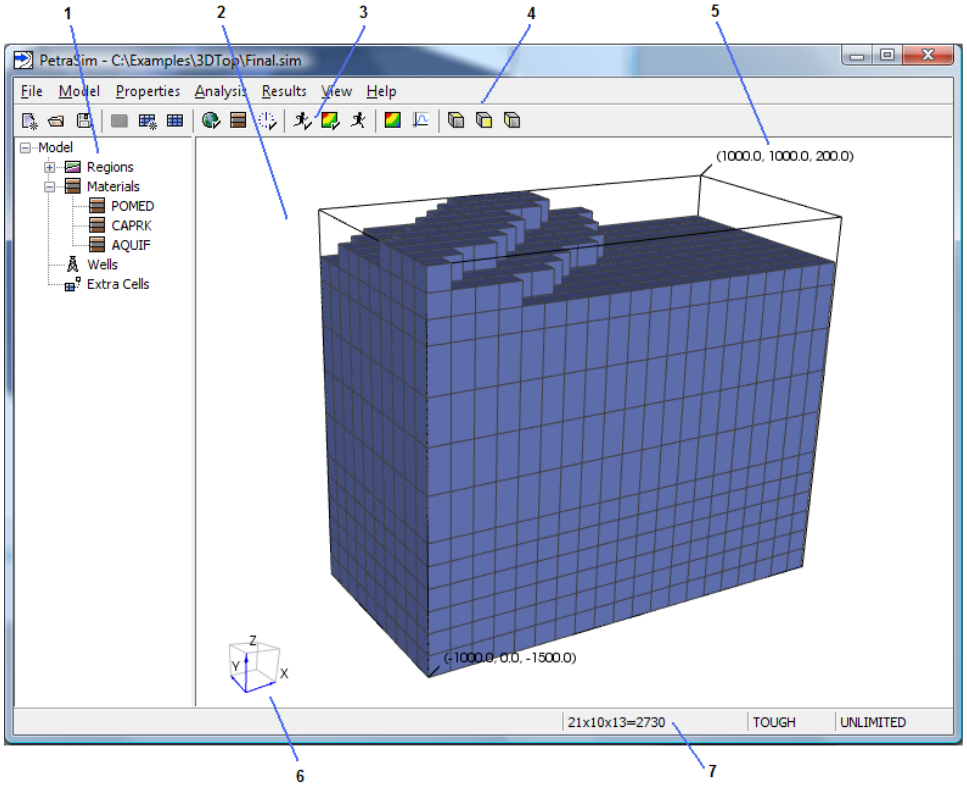

Figure 1.1. Main Window

1. **Navigation Tree** - Use this to quickly identify and manage items in your model.

2. **3D Model View** - Use this to visualize the structure of your model in 3D. When you use the Grid Editor, the current layer will be highlighted in this view.

3. **Toolbar** - The toolbar provides quick access to the steps required to define, run, and post-process an analysis.

4. **View** - Click to reset the 3D Model View to top, front, or side views.

5. **3D Labels** - Add 3D labels to help keep track of model features. Labels are added automatically when you add wells and when you create a model.

6. **Axis Legend** - To ensure that you never become disoriented, the axis legend rotates with your model and always displays the x, y, and z axes.

7. **Cell Count** - Use the cell count display to see how many cells are in your model.

2D Grid Editor

Use the 2D editor to specify properties for individual cells in your model. Examples of these properties include: initial conditions, enabling and disabling cells, and additional output data.

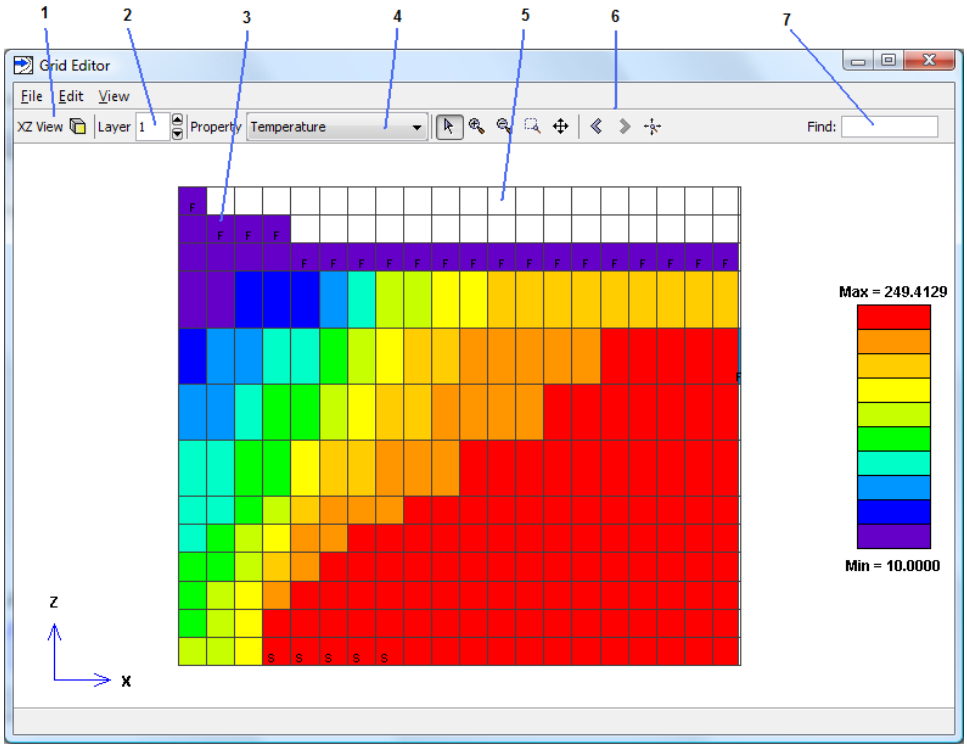

Figure 1.2. 2D Grid Editor

1. **View Selector** - Use this to switch between the three 2D viewing planes: XZ, XY, and YZ.

2. **Layer Selector** - Use this to select a layer of cells to edit. The currently selected layer is always highlighted in the Main Window.

3. **Cell Annotations** - Cells will display annotations when they are: a source or sink (S), fixed thermodynamic conditions (F), selected for additional output (P), or have been named.

4. **Property Selector** - Use this to color the current layer of cells based on a particular property such as temperature or gas saturation.

5. **Disabled Cells** - Cells that have been disabled will not be used in the simulation and are shown as empty in the Grid Editor.

6. **View** - Click this to undo, redo, or reset the view.

7. **Cell Finder** - To find any cell in the model, type either the name or the id number into this box, then press enter. The cell will be centered and selected in the Grid Editor.

3D Results View

You can use the 3D Results View to visualize properties of your model as they evolved over time.

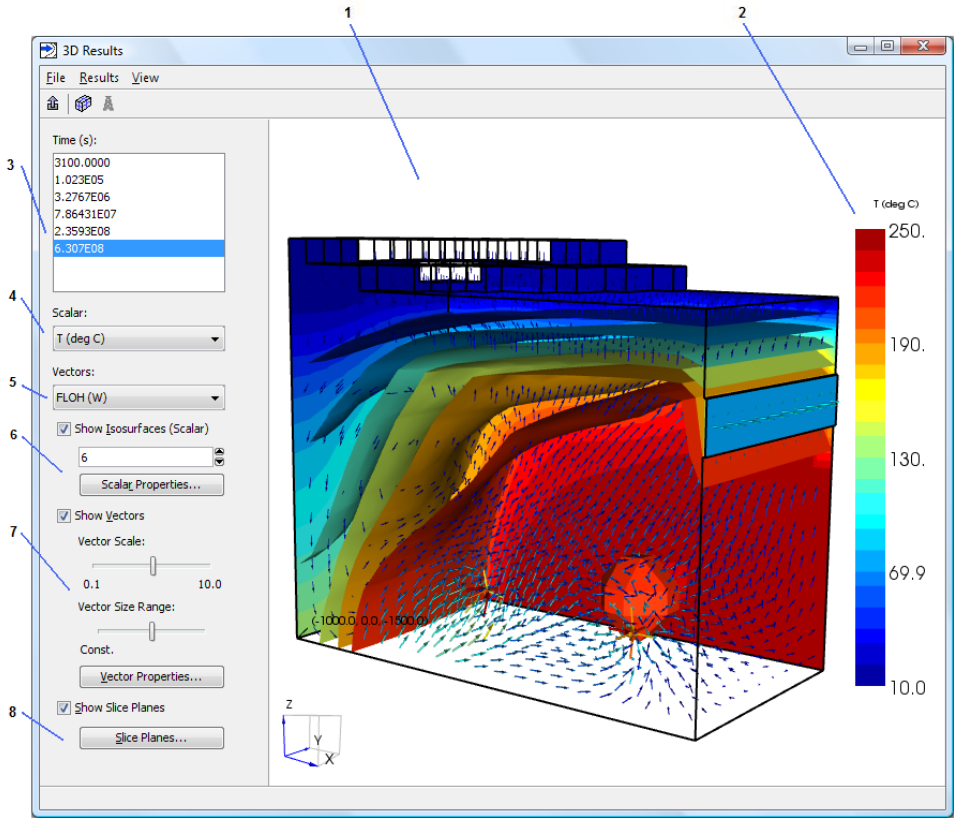

Figure 1.3. 3D Results View

1. **3D Results Display** - Contours, vectors, and slice planes are shown against an outline of your model. You can also make high-resolution screen shots for publications or presentation graphics.

2. **Scalar Legend** - The scalar legend shows what colors were used to display scalar quantities. You can also double-click the legend to define the range and number of colors.

3. **Time List** - Click a time step to view the results data at that time during the simulation.

4. **Scalar Property** - Select a scalar property, such as temperature or pressure) to display from this list. All slice planes and contours will be updated show the new property.

5. **Vector Property** - Select a vector property (such as water flow rate) to display from this list. All vectors will be updated to show the new property.

6. **Isosurface Controls** - Change the number of isosurfaces and and other scalar display properties.

7. **Vector Controls** - Use sliders to scale the vectors in the 3D view.

8. **Slice Planes** - Click this to add 2D slice planes to the 3D view.

Time History Results

You can make time history plots of individual cell data and export the data in a format for import into spreadsheets.

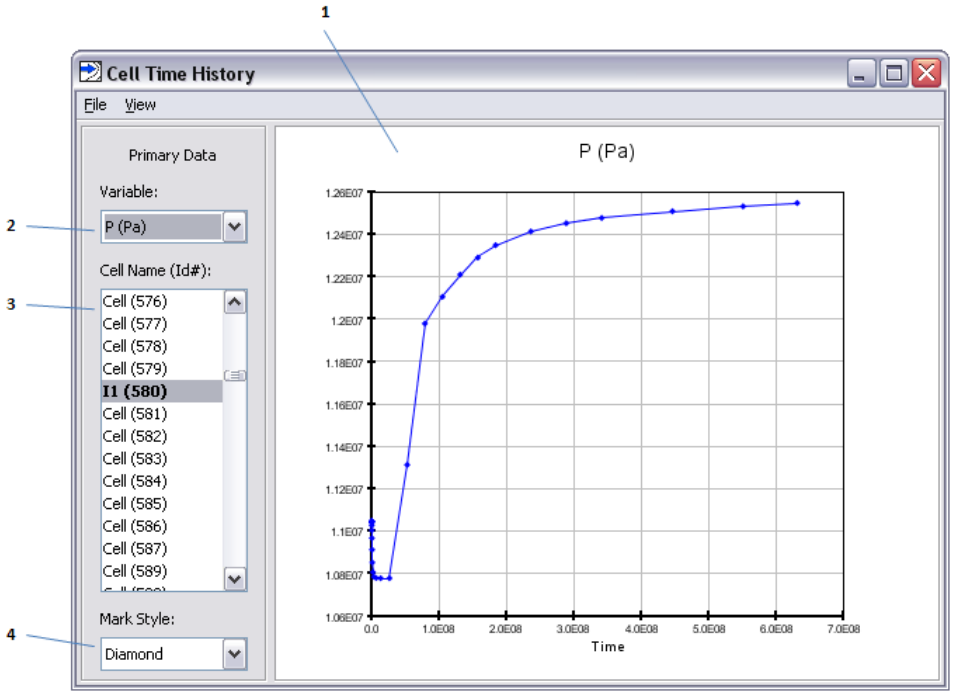

Figure 1.4. Time History Results

1. **Time History Results** - You can plot output data for any cell.

2. **Output Variable** - Select the output variable for plotting.

3. **Cell Selection** - Plots can be made for any cell. Named cells display the name and the cell number.

4. **Line Style** - Select the style for the graph.

Example Problems

PetraSim includes model files (*.sim) for each of the example problems in the C:\Program Files\PetraSim\samples directory. The examples can also be downloaded from the web at http://www.petrasim.com under the **Support** link.

PetraSim Tour (Five Spot)

This section is a (very) quick walkthrough for one of the sample problems included with TOUGH2. The problem specification is not discussed. You can just load the data, run the simulator, and look at the results. When you are ready, start PetraSim and follow the steps below.

Load the *eos1_five_spot* sample model

1. On the **File** menu, click **Open**
2. Select *c:\Program Files\PetraSim\samples\tough2\eos1_five_spot\five_spot.sim*, then click **Open**

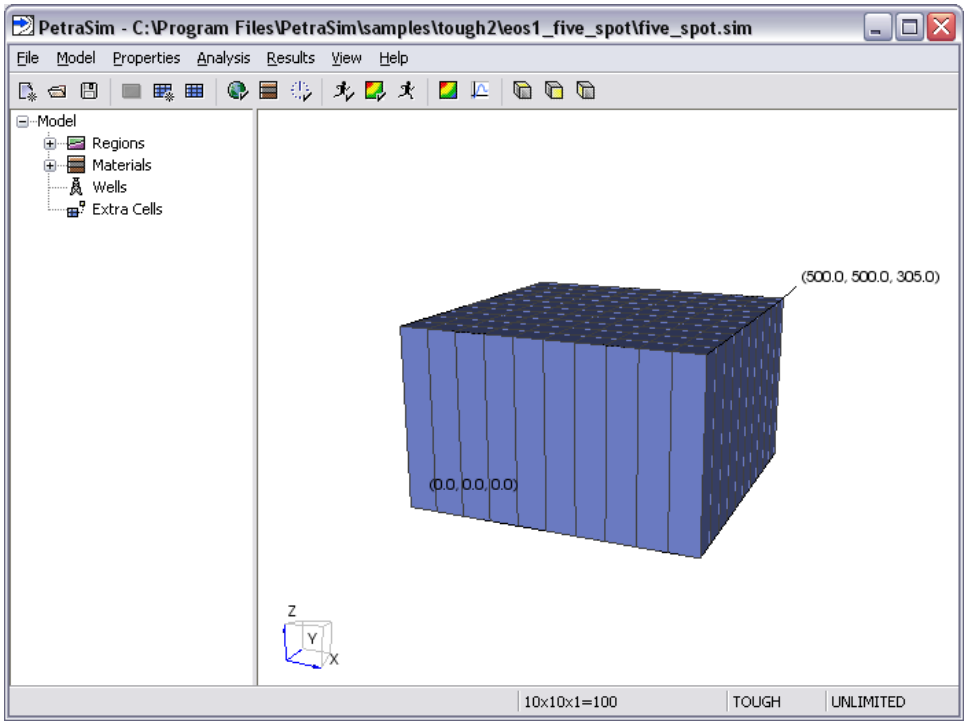

Figure 1.5. Opening the five spot model

Enable flux output

1. On the **Analysis** menu, click **Output Controls...**
2. Click to select **Fluxes and Velocities**
3. Click **OK**

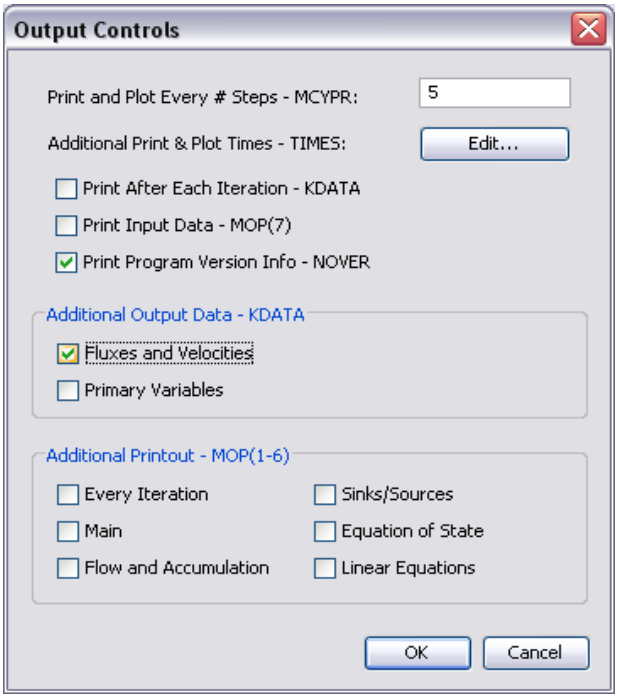

Figure 1.6. Select fluxes and velocities output

Run the simulation

To run the simulation: On the **Analysis** menu, click **Run TOUGH2**.

The Running TOUGH2 dialog will open and show how the simulation is progressing. The graph displays simulation time steps on the X-axis and the log10 of the time step on the Y-axis. As a rule of thumb, an increasing Y value is a good sign of simulation progress. If your time steps start to become smaller, it may indicate that the simulator is having a difficult time converging.

When the simulation finishes (approx 10 seconds), a message will be displayed and the Cancel button will turn into a Close button. Click the **Close** button.

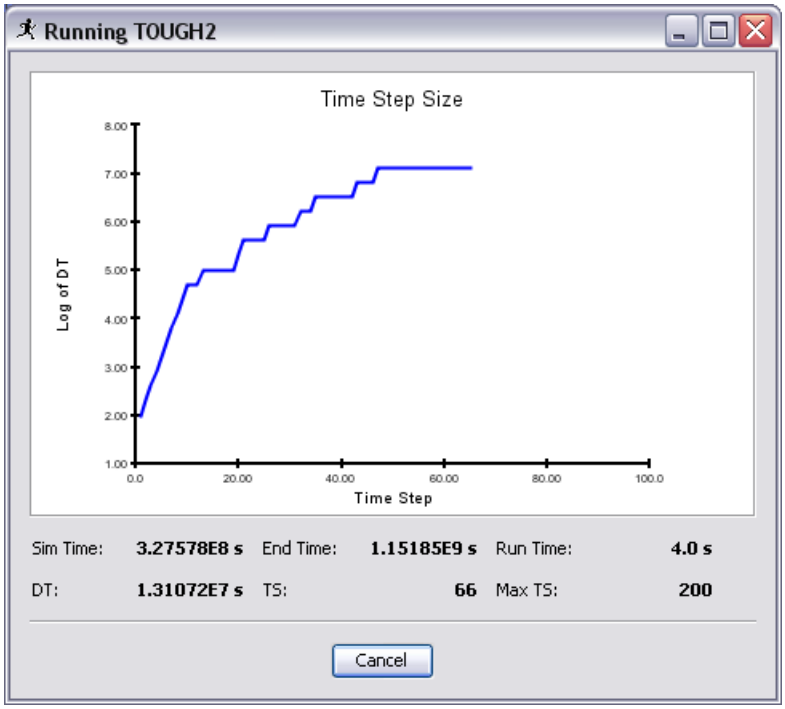

Figure 1.7. Time step graph during simulaton

View 3D simulation results

To view 3D simulation resuls: On the **Results** menu, click **3D Results...**.

Since this example problem is a 2D problem, it might be useful to add a scaling factor to the Z-axis. To scale an axis in the 3D Results:

1. On the **View** menu, click **Scale...**
2. Ini the **Z-Factor** box, type **0.01**
3. Click **OK**

The image below shows contour data for temperature and vectors for heat flow at the end of the simulation. When you are finished looking at the 3D results, close the 3D Results dialog and return to the PetraSim main window.

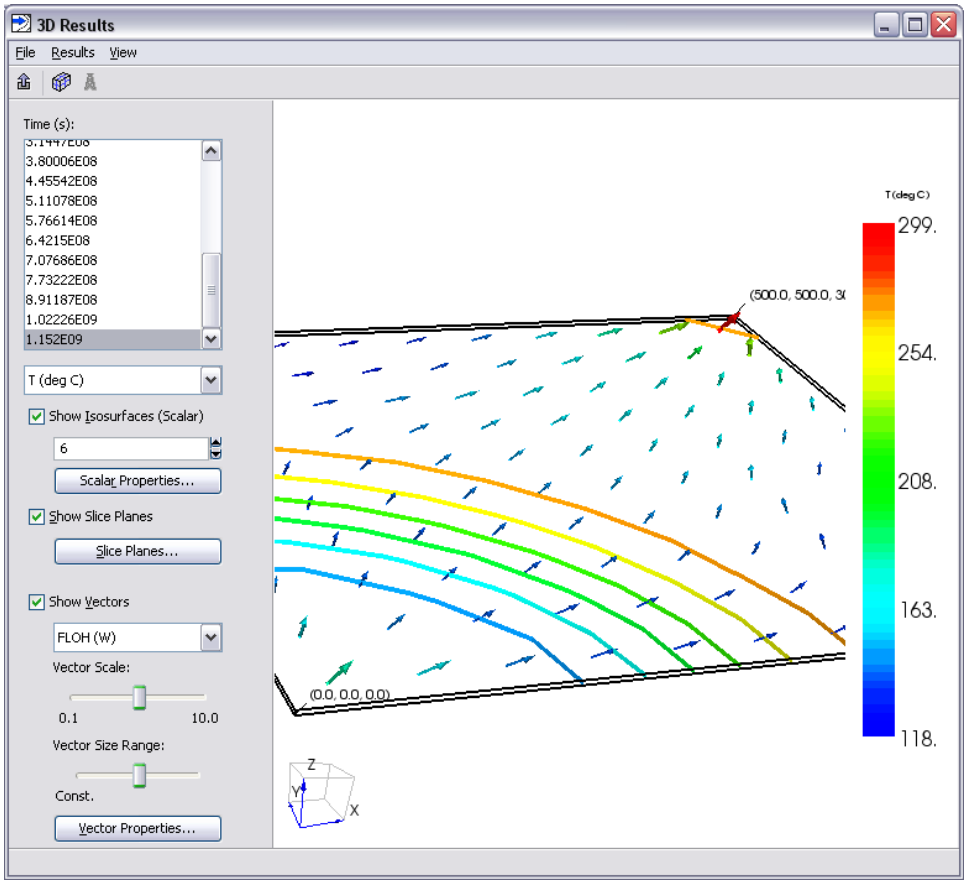

Figure 1.8. Temperature contours and flow vectors

View cell time history data

To open the cell time history view: On the **Results** menu, click **Cell History Plots**.

If you ask for additional time history data for some of your cells, they will appear in bold in the cell list. In this example, the injection and production cells were marked for additional output. These cells will have a data point for each time step of the simulation. You can view the time history of the rest of your cells by selecting the **Show All** option in the **View** menu.

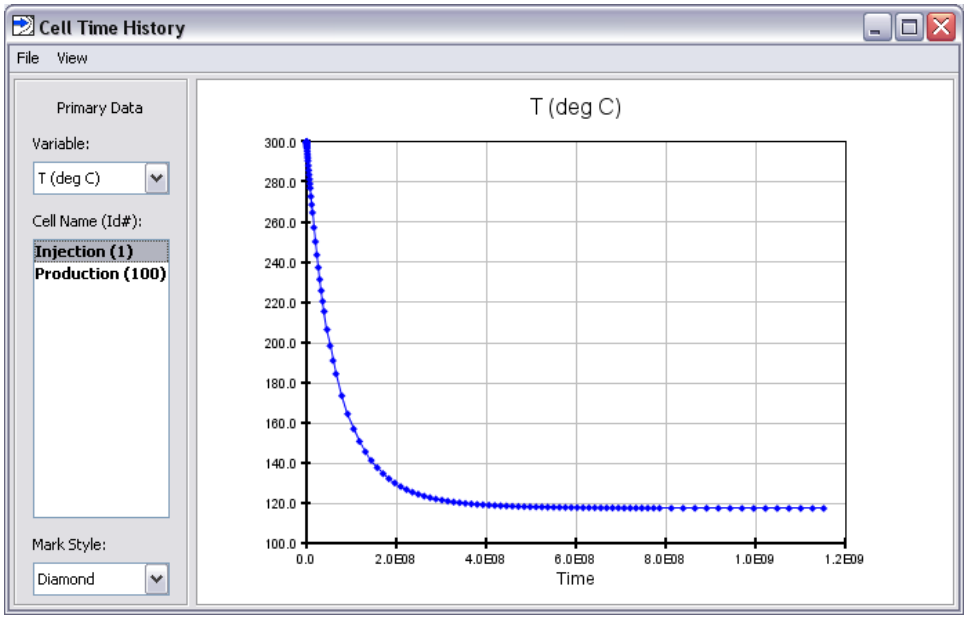

Figure 1.9. Temperature contours and flow vectors

Installation

PetraSim can be obtained at http://www.rockware.com/ by searching for "PetraSim" or at http://www.petrasim.com. To install, follow these instructions.

If running Windows NT, 2000, XP, or Vista, you must install PetraSim with administrator privileges. In addition, both the user and system must have read/write privileges to the installation directory (typically C:/Program Files/PetraSim). This requirement is placed by our licensing software.

From the web:

- Download the PetraSim setup.exe and save this file to disk.
- Double click on setup.exe to install.

From CD:

- Insert the CD in your CD-ROM drive and installation will begin automatically.
- If setup does not start automatically, click START on the taskbar and then click RUN. Type "D:\setup.exe" where "D:" is the drive letter for your CD-ROM.

30 Day Trial

After installation, you will be automatically registered for a 5 day trial period. To obtain a full 30 day trial version, you will need to obtain a new **Site Key**. On the **Help**

menu, click **Register...**. Copy and send the **Site Code** to <alison@rockware.com> or <support@thunderheadeng.com>. You will receive a **Site Key** which you will copy and paste into the **Site Key** box using the paste icon.

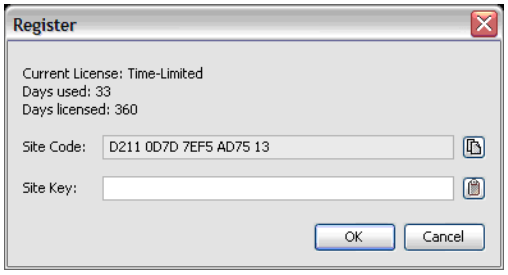

Figure 1.10. Registration dialog

Purchase of PetraSim

All PetraSim sales are handled by RockWare at http://www.rockware.com/. Our representative is Alison at <alison@rockware.com>. Search for "PetraSim" to go to the PetraSim sales page. Pricing for popular options are listed at the bottom of the page. Alison will provide a detailed quote at your request.

Registration

To register the software after purchase, on the **Help** menu, click **Register...**. Copy and send the **Site Code** to <alison@rockware.com>. You will receive a **Site Key** which you will copy and paste into the **Site Key** box using the paste icon.

Additional TOUGH Documentation

In preparing this manual, we have liberally used descriptions from the user manuals for the TOUGH family of codes. Links to download the TOUGH manuals are given at http://www.petrasim.com. More information about the TOUGH family of codes can be found at: http://www-esd.lbl.gov/TOUGH2/. Printed copies of the user manuals may be obtained from Karsten Pruess at <K_Pruess@lbl.gov>.

Computer Hardware Requirements

PetraSim will run well on any newer computer. At a minimum, the processor should be at least as fast as a 1 GHz Pentium III, with at least 512 MB RAM. A graphics card that supports OpenGL 1.1 or later with 64 MB of graphics memory is recommended.

Chapter 2. Flow in Porous Media

This section will provide only the briefest overview of the basic assumptions used in the TOUGH family of codes. The reader is referred to the TOUGH2 User's Guide [Pruess, Oldenburg, and Moridis, 1999], the T2VOC User's Guide [Falta, Pruess, Finsterle, and Battistelli, 1995], the TMVOC User's Guide [Pruess, Oldenburg, and Moridis, 1999], the TOUGHREACT User's Guide [Xu, Sonnenthal, Spycher, and Pruess, 2004], and the TOUGH-Fx/HYDRATE User's Guide [Moridis, Kowalsky, and Pruess, 2005] for detailed information on the TOUGH codes.

A good fundamental reference on flow in porous media is *The Physics of Flow Through Porous Media* [Scheidegger, 1957].

Darcy's Law for Single Phase Flow

The TOUGH family of codes (and thus PetraSim) simulate flow in porous media. A basic assumption is that the flow is described by Darcy's law,

$$\mathbf{u} = -\frac{k}{\mu}(\nabla p - \rho \mathbf{g})$$

where: $\mathbf{u}$ is the seepage velocity vector, k is total permeability, μ the viscosity, p the pressure, ρ the density, and $\mathbf{g}$ is the gravity vector.

Multi-Phase Flow

As described by Scheidegger [Scheidegger, 1957], when two (or more) immiscible fluids or phases exist simultaneously in a porous medium one phase will generally wet the solid. There are in general three saturation regimes:

- Saturation regime: The porous medium is completely saturated with one phase.
- Pendular regime: The porous medium has the lowest possible saturation with one phase. This phase occurs in the form of pendular bodies throughout the porous medium. These pendular bodies do not touch each other so that there is no possibility of flow for that phase, see Figure 2.1.a.
- Fenicular regime: The porous medium exhibits an intermediate saturation with both phases. If the pendular bodies of the pendular regime expand through addition of the corresponding fluid, they eventually become so large that they touch each other and merge. The results is a continuous network of both phases across the porous medium. It is thus possible that simultaneous flow of both phases occurs along tortuous paths, see Figure 2.1.b.

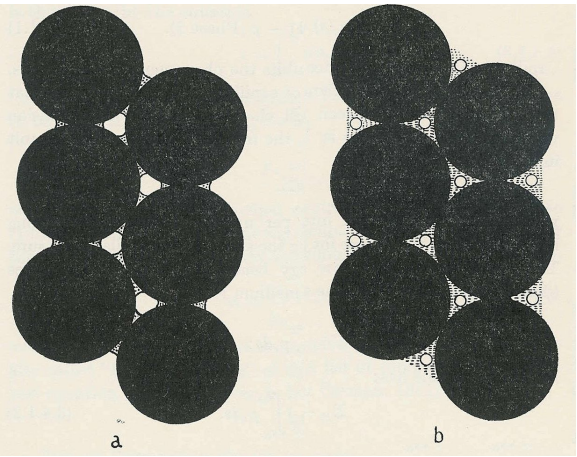

Figure 2.1. Illustration of pendular (a) and funicular (b) saturation regime in the case of an idealized porous medium consisting of packed spheres [Versluys, 1931]

For multi-phase flow, Darcy's law is modified to introduce the concept of relative permeability:

$$\mathbf{u}_\beta = -k\frac{k_{r\beta}}{\mu_\beta}\left(\nabla p_\beta - \rho_\beta \mathbf{g}\right)$$

Where β indicates the phase, $k_{r\beta}$ is the relative permeability (between 0 and 1) for the phase, and

$$p_\beta = p + p_{c\beta}$$

is the fluid pressure in the phase, which is the sum of the pressure in a reference phase (usually the gas phase) and the capillary pressure $p_{c\beta}$ (capillary pressure is negative).

Relative Permeability

The TOUGH codes provide several options for relative permeability. A typical option is the use of Corey's curves [Corey, 1954] as illustrated in Figure 2.2. At low liquid saturation, the gas relative permeability is 1.0 and the liquid permeability is very low. Conversely, at high liquid saturation the gas relative permeability is very low and the liquid permeability is 1.0. This is consistent with the flow regimes as described above.

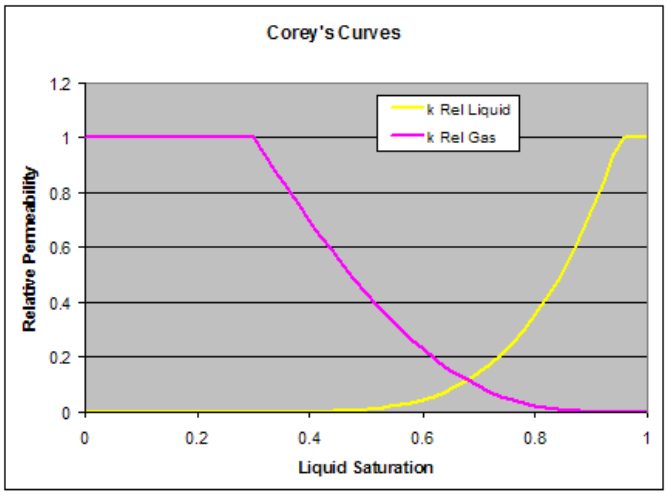

Figure 2.2. Relative permeability using Corey's curves

Capillary Pressure

The TOUGH codes also provide several options for capillary pressure. A typical option is the van Genuchten function [van Genuchten, 1980] as illustrated in Figure 2.3. At low liquid saturation, the capillary pressure is large, but rapidly becomes smaller as liquid saturation increases.

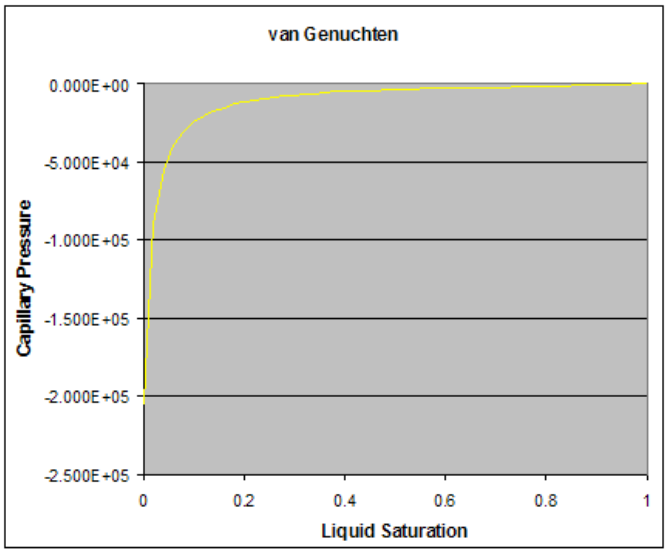

Figure 2.3. Capillary pressure using van Genuchten function

Chapter 3. TOUGH Concepts

Components and Phases

A clear understanding of the terms **component** and **phase** is necessary when using the TOUGH codes. Consider a system consisting of water and air (implemented as EOS3 in TOUGH2). This system consists of two components (water and air) and will have two phases (liquid and gas). Note that TOUGH2 does not include a solid phase, which would consist of ice; TOUGH-Fx/HYDRATE does include ice as a solid phase.

Importantly, the two components (water and air) can be present in both phases. The liquid phase can consist of liquid water **and** dissolved air. Similarly, the gaseous phase can be comprised of gaseous air **and** water vapor.

For single phase conditions, the thermodynamic state is defined by pressure, temperature, and air mass fraction. If the single phase is liquid, then the air mass fraction will be the air dissolved in the water, which is a small value. An example of a valid initial condition specification for single phase liquid is shown in Figure 3.1, with pressure of 1.0E5 Pa, temperature of 20 C, and a small air mass fraction of 1.0E-5. This small amount of air will be dissolved in the water.

If the single phase is gas, the gas can consist of both water vapor and air. The air mass fraction can be as large as 1. A valid initial condition specification for single phase gas is given in Figure 3.2, with pressure of 1.0E5 Pa, temperature of 20 C, and a air mass fraction of 0.999. This means that a small amount of the gas will consist of water vapor.

For two phase conditions, the thermodynamic state is defined by gas phase pressure, gas saturation, and temperature. An example of a two phase initial condition is given in Figure 3.3, with pressure of 1.0E5 Pa, temperature of 20 C, and gas saturation of 0.5.

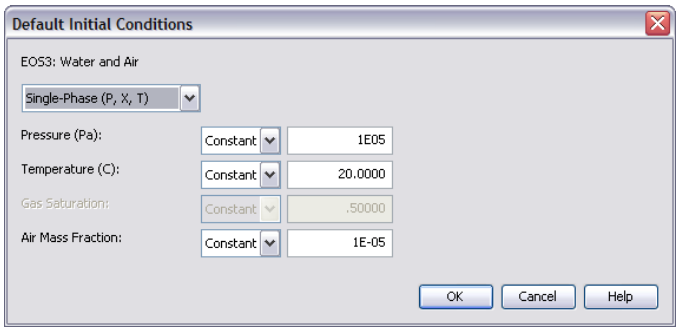

Figure 3.1. Single phase liquid initial conditions for EOS3

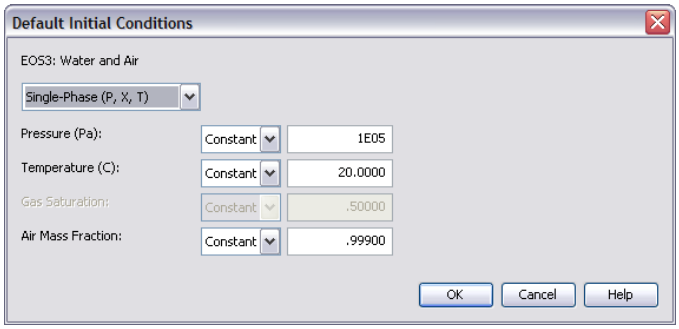

Figure 3.2. Single phase gas initial conditions for EOS3

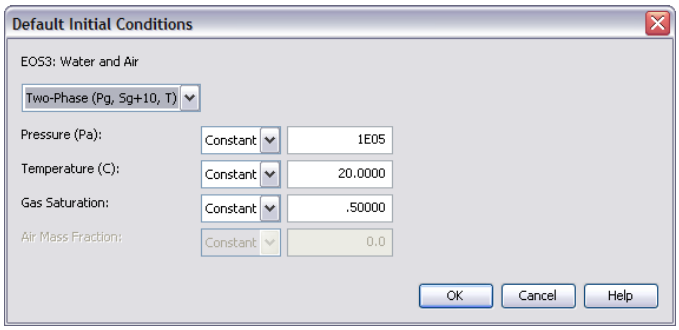

Figure 3.3. Two phase initial conditions for EOS3

As an example, a single element with a volume of 1 cubic meter and 0.1 porosity was run using the initial conditions given above. The resulting solution and mass fractions for each component are given below, in Figure 3.4 and Figure 3.5. The two phase solution is of particular interest since this case provides the saturation conditions for water vapor in the gas phase and dissolved air in the liquid phase. The reader is encouraged to use single element problems when starting to use a new equation of state (EOS).

State	P (Pa)	T (C)	Gas Saturation	Liquid Saturation	Mass Frac. Air in Gas	Mass Frac. Air in Liq.	Perm. Modifier	Density Gas	Density Liquid
Single Phase Liquid	1.000E+05	20.000	0.000	1.000	0.000	0.000	1.000	0.000	998.320
Single Phase Gas	1.000E+05	20.000	1.000	0.000	0.999	1.605E-05	1.000	1.187	0.000
Two Phase	1.000E+05	20.000	0.500	0.500	0.985	1.570E-05	1.000	1.177	998.300

Figure 3.4. States corresponding to the three initial condition options

State	Phase Volumes in Place (m^3)		Mass in Place (kg)				
	Gas	Liquid	Gas	Liquid	Air	Vapor	Liquid Water
Single Phase Liquid	0.000	0.100	0.000E+00	9.983E+01	9.983E-04	0.000E+00	9.983E+01
Single Phase Gas	0.100	0.000	1.187E-01	0.000E+00	1.186E-01	1.187E-04	0.000E+00
Two Phase	0.050	0.050	5.888E-02	4.992E+01	5.880E-02	8.645E-04	4.992E+01

Figure 3.5. States corresponding to the three initial condition options

In TOUGH2, all water properties are represented by the steam table equations as given by the International Formulation Committee [International Formulation Committee, 1987]. Air is approximated as an ideal gas, and addititivity is assumed for air and vapor partial pressures in the gas phase. The viscosity of air-vapor mixtures is computed from a formulation give by Hirshfelder et al. [Hirschfelder et al., 1954]. The solubility of air in liquid water is represented by Henry's law.

Because of the detailed physics that are included in the TOUGH codes, setting of multi-phase initial conditions requires detailed understanding of the problem. For help in setting mixture conditions, the user may refer to a thermodynamics text, such as [Cengel and Boles, 1989].

Mass and Energy Balance

As described in the TOUGH2 manual, the basic mass and energy balance equations solved by TOUGH2 can be written in the general form:

$$\frac{d}{dt}\int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n}\, d\Gamma_n + \int_{V_n} q^{\kappa} dV_n$$

The integration is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_n. The quantity M appearing in the accumulation term (left hand side) represents mass or energy per volume, with κ labeling the mass components and an extra heat "component" if the analysis is nonisothermal. $\mathbf{F}$ denotes mass or heat flux and q denotes sinks and sources. $\mathbf{n}$ is a normal vector on surface element $d\Gamma_n$, pointing inward to V_n.

The user should consult Appendix A of the TOUGH2 User's Guide [Pruess, Oldenburg, and Moridis, 1999] for a further discussion of this topic.

Spatial Discretization

As described in the TOUGH2 User's Manual, the continuum equations are discretized in space using the integral finite difference method (IFD), [Edwards, 1972] and [Narisham and Witherspoon, 1976]. Introducing appropriate volume averages, we have

$$\int_{V_n} M\, dV = V_n M_n$$

where M is a volume-normalized extensive quantity, and M_n is the average value of M over V_n. Surface integrals are approximated as a discrete sum of averages over surface segments A_{nm}:

$$\int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n}\, d\Gamma_n = \sum_m A_{nm} F_{nm}$$

Here F_{nm} is the average value of the (inward) normal component of F over the surface segment A_{nm} between volume elements V_n and V_m. The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Figure 3.6.

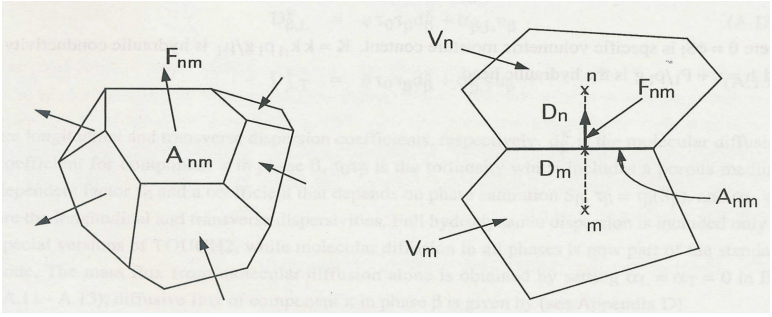

Figure 3.6. Space discretization and geometry data in the integral finite difference method (from TOUGH2 User's Guide)

The discretized flux is expressed in terms of averages over parameters for elements V_n and V_m. For the basic Darcy flux term, we have

$$F_{\beta,nm} = -k_{nm}\left[\frac{k_{r\beta}\rho_\beta}{\mu_\beta}\right]_{nm}\left[\frac{P_{\beta,n}-P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}g_{nm}\right]$$

where the subscripts (nm) denote a suitable averaging at the interface between grid blocks n and m (interpolation, harmonic weighting, upstream weighting). $D_{nm} = D_n + D_m$ is the distance between the nodal points n and m, and g_{nm} is the component of gravitational acceleration in the direction from m to n.

The user should consult Appendix B of the TOUGH2 User's Guide [Pruess, Oldenburg, and Moridis, 1999] for a further discussion of this topic.

Temporal Discretization

Substituting the volume averaged quantities and surface integral approximations into the mass and energy balance, a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_n^\kappa}{dt} = \frac{1}{V_n}\sum_m A_{nm}F_{nm}^\kappa + q_n^\kappa$$

Time is discretized as a first order finite difference, and the flux and sink and source terms on the right-hand side are evaluated at the new time, to obtain the numerical stability needed for an efficient calculation of multiphase flow.

The user should consult Appendix B of the TOUGH2 User's Guide [Pruess, Oldenburg, and Moridis, 1999] for a further discussion of this topic.

Chapter 4. Equations of State

As described in the TOUGH2 User's Guide, the thermophysical properties of fluid mixtures needed for assembling the governing mass- and energy-balance equations are provided by "equation-of-state" (EOS) modules. Each equation of state uses a different set of primary variables (such as pressure, temperature, and mass fractions) to define each possible phase condition. When the phase changes, the EOS switches and initialized new primary variables.

PetraSim supports the following EOS options in TOUGH2, Figure 4.1. PetraSim also supports TOUGHREACT, TMVOC, and TOUGH-Fx/HYDRATE. For the options available for these different versions, go to **File->Preferences...**.

EOS	Description
1	Water, water with tracer
2	Water and CO_2
3	Water and air
5	Water and hydrogen
7	Water, brine, and air
7R	Water, brine, two radionuclides, and air
9	Saturated-unsaturated flow (used for vadose zone)
EWASG	Water, NaCl, non-condensible gas
ECO2	Water, brine, and CO2 for sequestration studies

Figure 4.1. States corresponding to the three initial condition options

Selecting an EOS

To select an EOS, go to **File->Preferences...**. On this dialog, you can select the TOUGH version and a particular EOS supported by that version. After making the selection, you must then select **File->New** to create a new model with the new EOS. Your preference will be remembered by PetraSim, so that next time you create a new model, it will start with the EOS you previously selected as your preference.

There can be only one EOS in an analysis.

Global Properties

Each EOS has different options that define the assumptions used in the analysis. For EOS3, this includes whether to include heat transfer (isothermal or non-isothermal) and whether to include molecular diffusion. These options are selected by selecting **Properties->Global Preferences...** or on the toolbar. On the **EOS** tab all available options will be displayed.

Details for Each EOS

The user is referred to the TOUGH2 User's Guide [Pruess, Oldenburg, and Moridis, 1999] for detailed descriptions of the options available for each EOS.

Chapter 5. PetraSim Basics

Work Flow in a Typical Analysis

Many problems will be run in two stages: (1) an analysis that establishes a steady state initial condition, and (2) an analysis that loads the steady state results as an initial condition and then proceeds with a transient disturbance, such as a spill or production from a reservoir. PetraSim makes it easy to load the results of a previous analysis as the starting condition of a new analysis.

The PetraSim interface helps guide the user through the steps of an analysis. These include:

- Selecting an EOS.
- Defining the problem boundaries and creating a mesh.
- Selecting the global options to be used in the analysis.
- Specifying the material properties.
- Defining the default initial conditions for the model, either directly or by loading the results of a previous analysis.
- Using the grid editor to define cell-specific data, such as material, sources, sinks, and initial conditions.
- Setting the solution and output options.
- Solving the problem.
- Post-processing of results using contour and time history plots.

The user must recognize that this process is seldom linear. It will likely be necessary iterate as new understanding of the model and physics is obtained. New users are especially tempted to immediately proceed with a complex model. Don't do this! It is always recommended that the user perform a 1D and 2D analyses before a 3D analysis.

A suite of examples taken from the TOUGH user guides is available at http://www.petrasim.com/.

PetraSim Interface

PetraSim uses multiple views to display the model and results:

- 3D View. Used to rapidly view the model, including internal boundaries and wells.
- Tree View. Used to display and select regions in the model, materials, wells, and extra cells.

- Grid Editor. Used to define cell-specific parameters including sources and sinks and initial conditions.
- 3D Plots. Used to display isosurfaces and contour plots of results.
- Time History Plots. Used to display detailed cell results as a function of time.

3D View

To navigate using the 3D model:

- To **spin** the 3D model **left-click** on the model and move the mouse. The model will spin as though you have selected a point on a sphere.
- To **zoom**, hold the **Alt** key and drag the mouse vertically.
- To **move** the model, hold the **Shift** key and drag to reposition the model in the window.
- To **reset** the model, type "r" or select .
- To change to a standard view, select for a **top** view, for a **front** view, and for a **side** view.

Grid Editor (2D View)

The Grid Editor is used to make cell-specific changes to the model. Select **Model->Edit Grid** or to open the grid editor.

The Grid Editor will display a section through the model, Figure 5.1. To change the properties of a cell, either select the cell and then **Edit->Properties** or right-click on the cell.

In the toolbar, you can select the viewing direction, the grid layer, and the property to be plotted. Tools include **selection** , **zoom in** , **zoom out** , **zoom box** , **drag** , **previous view** , **next view** , and **reset** .

To help with orientation in the model, the layer being viewed in the Grid Editor is highlighted in the 3D View, Figure 5.2.

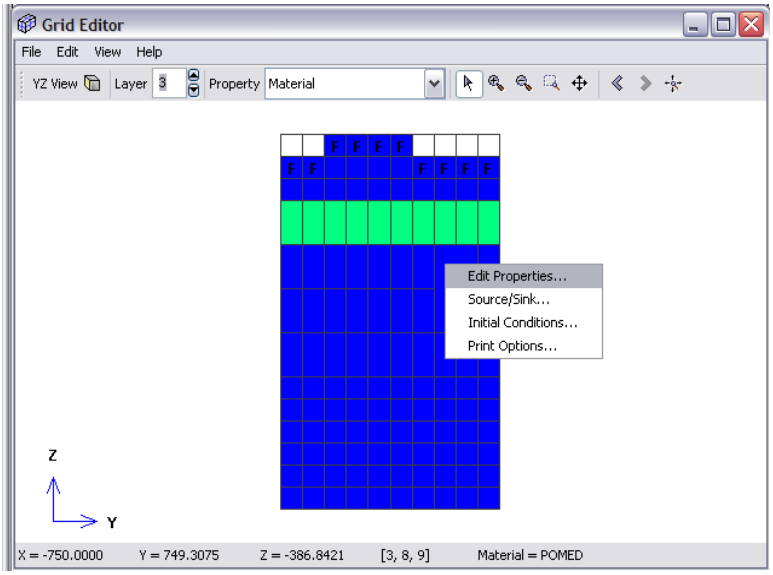

Figure 5.1. The grid editor view

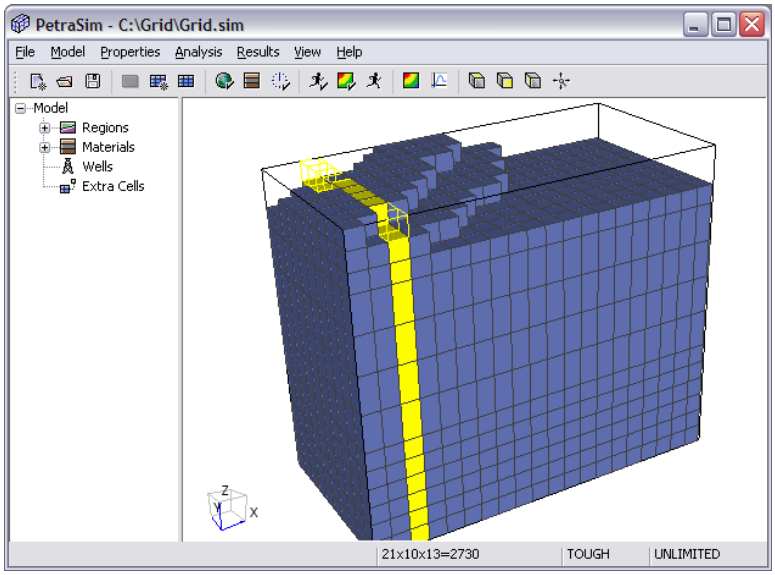

Figure 5.2. The 3D view showing which cell layer is being edited in the Grid Editor

Tree View

The Tree View (on the left of the 3D window) is used to display and select regions, materials, wells, and extra cells. Expand the list and then double-click on an object to edit its properties.

Enabled, Disabled, and Fixed State Cells

In the Grid Editor, the Properties of a cell can be set to Type **Enabled**, **Disabled**, or **Fixed State**, with the following meanings:

- An Enabled cell is a standard cell in the analysis.
- A Disabled cell will not be included in the analysis. No information about this cell will be written to the TOUGH input file. It will not be included in the results.
- An Fixed State cell is used to set boundary conditions. The cell is included in the analysis, but the state of the cell (Pressure, Temperature, etc.) will not change. In the TOUGH2 User's Guide, such cells are named "Inactive". It was necessary for us to use a different name to distinquish between Fixed and Disabled cells.

Units

All input uses standard metric (SI) units, such as meters, seconds, kilograms, degrees C, and the corresponding derived units, such as Newton, Joules, and Pascal for pressure.

Contour Data

Externally generated contour data can be used to define 3D inital conditions or to define the topology of the top and bottom of the model. This data is read from a contour file.

The format of the contour file is given below; it follows that used by TETRAD. The contour data can be viewed as a set of planes on which contours are defined. The planes can be defined at several depths in the model, forming a complete 3D definition of the data. Linear interpolation is performed in the Z direction between the contour planes.

The data consists of the depth (Z coordinate) followed by a definition of contours at that depth. In the following example, the "!" and following comments are included only for description. These should not be included in an actual file.

```
Define top of reservoir    ! The first line is a description
<top origin>               ! Include this line (not used at this time)
<depth>                    ! Keword to indicate beginning of a contour set
    0.                     ! The Z coordinate for this contour set
<contour>                  ! Keyword to define a contour at the given depth
    0.     1               ! Value of contour followed by number of points
-1000.  1000.              ! X and Y coordinates of the point(s)
<contour>                  ! Start of a new contour
  200.     3               ! Value (200.0) and number of points (3)
 -100. 1000.               ! X and Y coordinates of the point(s)
 -300.  800.               ! X and Y coordinates of the point(s)
-1000.  200.               ! X and Y coordinates of the point(s)
<contour>                  !
  100.     4               ! Complete the contours at this depth.
  200. 1000.
    0.  600.
 -400.  200.
 -800.    0.
<contour>
    0.     4
  400. 1000.
```

```
  200.  600.
 -200.  200.
 -600.    0.
<contour>
    0.     2
 1000.    0.
 1000. 1000.
                              ! Repeat <depth> and <contour> data
```

Chapter 6. Working with Files

Several files are used when performing an analysis using PetraSim. These include the PetraSim model file, the TOUGH input file, and TOUGH output files. It is important to understand the differences between these files to take full advantage of PetraSim's features

PetraSim Model File

The PetraSim model file (*.sim) is a binary file that completely represents a PetraSim model. The PetraSim model contains all information needed to write a TOUGH input file.

The PetraSim model file (*.sim) should be used to save the model and share with other PetraSim users.

TOUGH Input File

Execution of TOUGH is integrated into PetraSim. Before PetraSim executes TOUGH, an TOUGH input file (*.dat) is automatically written. This file is then read by the TOUGH executable. The TOUGH input file contains all information needed for an TOUGH analysis. The FDS input file is an ASCII file.

Most PetraSim users will never need to explicitly create or edit the TOUGH input file. In special cases, such as when a user has developed a special version of TOUGH, the user may need to edit the TOUGH input file before an analysis. In this case, PetraSim provides the option to export this file (**File/Export/TOUGH File...**) for manual editing.

PetraSim users should not use the TOUGH file to share models, since extra model information that is included in the PetraSim model file will be lost.

Creating and Saving a New PetraSim Model

When PetraSim is started, it begins with an empty model. The user can immediately begin work on a new model. If another model has already been opened, select **File->New...** to clear the current model and start a new empty model. PetraSim always has one (and only one) active model.

To save the new model, select **File->Save...** and give the file name. Because the files written by TOUGH have a fixed name, it is recommended that the user create a new directory for each model. If this is not done, the TOUGH results from a first analysis will lost when a second model is run, even if the PetraSim model has a different name.

Open a Saved PetraSim Model

To open a saved model, select **File->Open...** and select the file. To speed model selection, a list of recently opened files is available under **File->Recent PetraSim Files...**.

Chapter 7. The Solution Grid

Problem Boundary

The first step in creating a model is to define the boundary. Select **Model->Define Boundary...** or to open the Define Model Boundary dialog, Figure 7.1. In this dialog, give the grid dimensions and select the material to be used as the default material for the model.

If the model is to be an RZ axisymmetric model, then set Y min to 0.0 and Y max to 1.0.

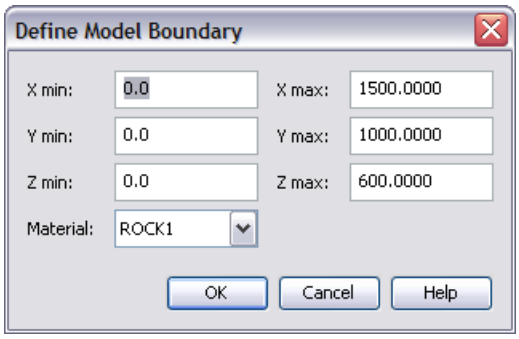

Figure 7.1. Defining the boundary of the model

Internal Boundary

Internal boundaries can be used to divide a model into regions. Material properties and initial conditions can then be defined by region. Select **Model->Add Internal Boundary...** or to open the Add Internal Boundary dialog, Figure 7.2.

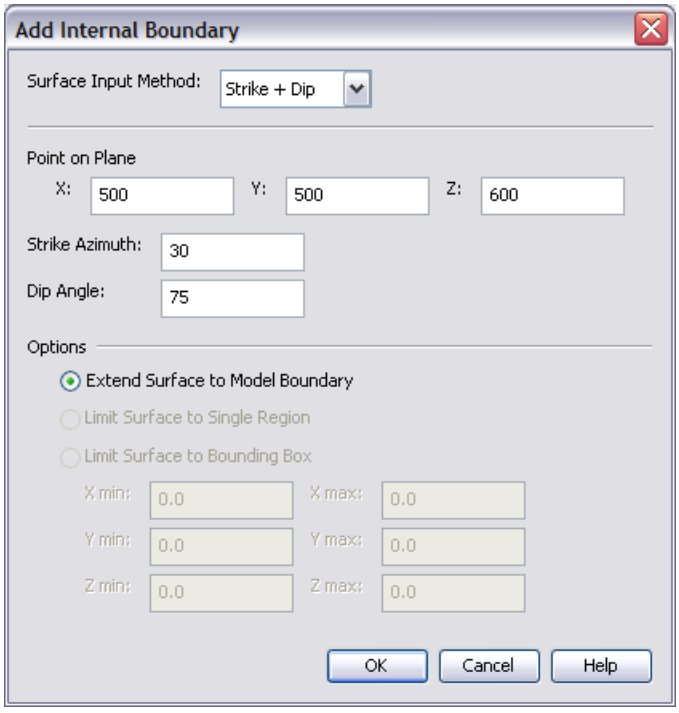

Figure 7.2. Defining an internal boundary

The internal boundary is a plane that extends to the boundary of the model. Several options: Strike + Dip, Three Points, and Point + Normal are provide to define this plane. Figure 7.2 shows the input using the Strike + Dip option. The resulting internal boundary is shown in Figure 7.3.

For the **Strike + Dip** option, the data include:

- Point on Plane - The coordinates of a point on the boundary plane.
- Strike Azimuth - The degrees from North (the positive Y axis) in a clockwise direction.
- Dip Angle - Degrees from horizontal of the plane. If the viewer is facing the azimuth direction, the dip is to the viewer's right.

For the **3 Points on a Plane** option, the data include:

- Points on Plane - The coordinates of three points on the boundary plane.

For the **Point + Normal** option, the data include:

- Point on Plane - The coordinates of a point on the boundary plane.
- Normal to Plane - The components of a vector normal to the plane. They do not

need to be normalized.

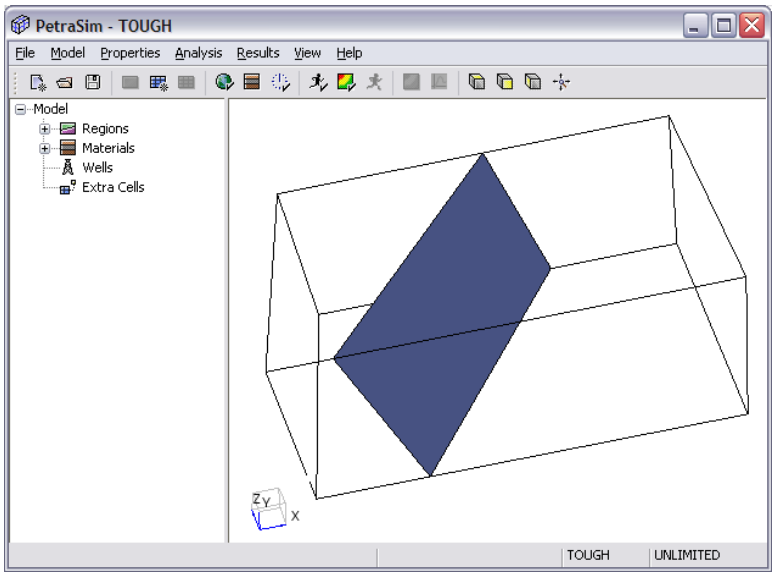

Figure 7.3. The internal boundary shown in the model

You can now use the mouse (or Tree View) to select a region and define a material or initial condition to that region. PetraSim uses a hierarchy when writing the TOUGH input file properties for a cell. If a property has been defined for a specific cell in the Grid Editor, that is used. Next, the region in which the cell lies is used to define properties. Finally, the default model properties are used.

Top and Bottom Surfaces

PetraSim has the capability to define the topography of the top and bottom of the model. Any cell whose center is above the top or below the bottom surface will be disabled (not included in the analysis).

Boundaries are useful if the user is modeling the surface of the earth or a deposit that varies with depth. Three options can be used to define the top and bottom surfaces: a constant Z depth, a linear function, or a contour file. The format of the contour file is described in the chapter "Petrasim Basics." Contour files for download are provided with the example manual.

To define the surface, select **Model->Set Top and Bottom...**. In the Set Top and Bottom dialog choose the option for defining the surfaces, Figure 7.4.

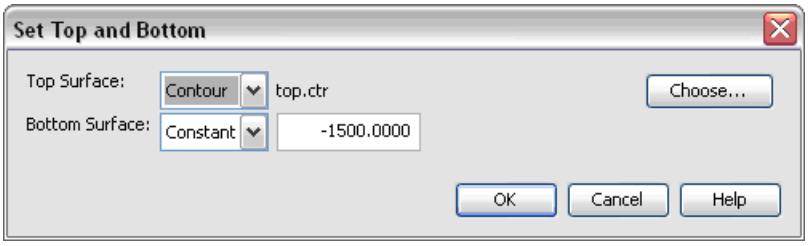

Figure 7.4. Defining the top and bottom surfaces of the model

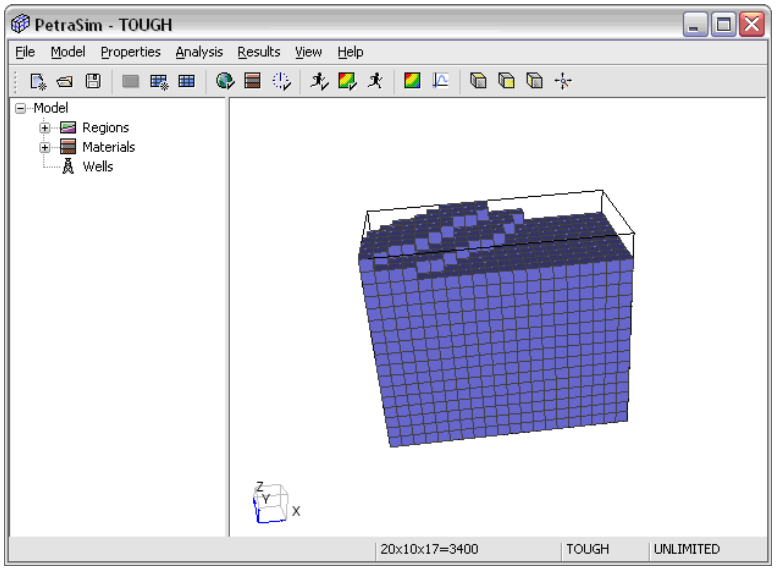

Figure 7.5. Model with top surface defined

Creating Solution Grids

The solution grid is the discretization used to solve the analysis. You have the option of creating a "regular" grid or a "Meshmaker" grid. In a regular grid, the cell sizes are uniform or increase geometrically. In a Meshmaker grid, the size of each cell is specified.

Select **Model->Create Grid...** or to open the Create Grid dialog, Figure 7.6.

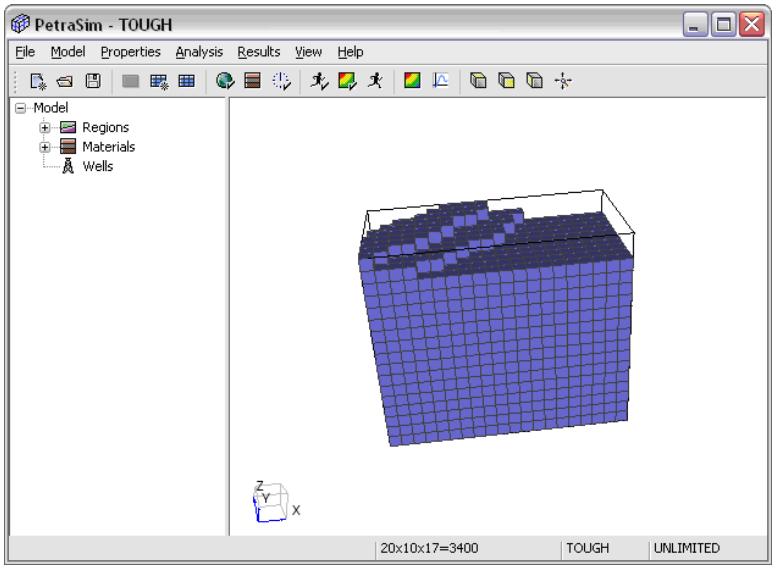

Figure 7.6. The Create Grid dialog

Regular Grid

If top or bottom surfaces have been defined, the user is provided two options: either to disable cells above and below the top and bottom or to shift the grid to conform to the top and bottom. The first option is recommended, since it preserves the convergence properties of the rectangular grid. However, the shifted grid is an option that is often used in reservoir models if the flow is primarily in the XY plane. It uses the cells efficiently and the error introduced is usually relatively small.

The user can also select an XYZ (full 3D) or RZ (axisymmetric) grid. If the RZ grid option is selected, then there will be only one layer of cells in the Y direction. The model will be displayed as a plane, however, when the cell data is written for the solution, the correct cell volumes and connection areas are calculated that represent an axisymmetric model.

The required input is the number of cells in each direction and a factor used to increase or decrease element size. If the factor is 1.0, then all cells in that direction have the same size. If not, the relations in Figure 7.7 can be used to calculate the cell size that will result for a given initial size and factor.

$$l = l_0 + l_1 + l_2 + \ldots + l_{n-1}$$
$$l = l_0 f^0 + l_0 f^1 + l_0 f^2 + \ldots + l_0 f^{n-1}$$
$$l = l_0 \sum_{i=0}^{n-1} f^i$$

Figure 7.7. Calculating cell size when the factor is not 1.0

Meshmaker Grid

The user defines the size of each cell when creating a Meshmaker grid. The cells are defined in the direction of increasing coordinate (X, Y, or Z) and the user gives the direction, number of cells, and size of those cells. This must be defined for each direction and the sum of all cell sizes must match the boundary length in each direction.

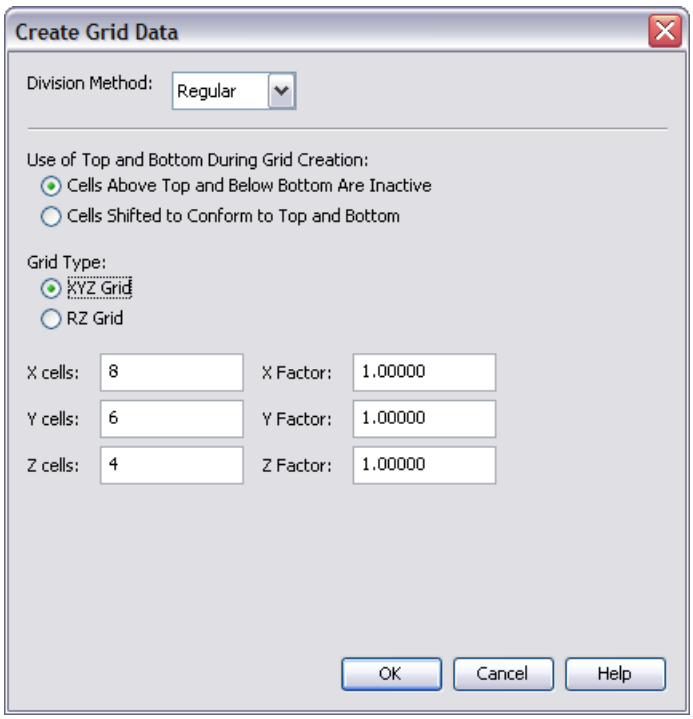

Figure 7.8. Using the Meshmaker option to create a grid

Editing a Cell

The user can edit the properties of a cell in the Grid Editor. Open the Grid Editor and right-click on a cell to display the context menu, xref linkend="Cell_01" xrefstyle="select: label"/>. Select Properties, Figure 7.10. The user provides:

- Cell Name - A decriptive name that can be used to access cell results for plotting.
- Cell ID - This is calculated by PetraSim, not editable.
- X, Y, and Z Center - The center of the cell, not editable.
- Volume - The volume of the cell.
- Volume - The volume of the cell calculated based on dimensions, not editable.
- Volume Factor - A multiplier on the volume that is used to obtain the final volume sent to the TOUGH input file.

- Material - The material for the cell.
- Type - Enabled (included as standard cell), Disabled (not included in analysis), or Fixed State (set as fixed boundary condition). See PetraSim Basics for further details.
- Z Thickness - Allows the user to change the Z dimension of the cell. This is calculated by PetraSim for "shifted Z" grids.
- Z Base - Allows the user to change the Z coordinate of the base of the cell. This is calculated by PetraSim for "shifted Z" grids.

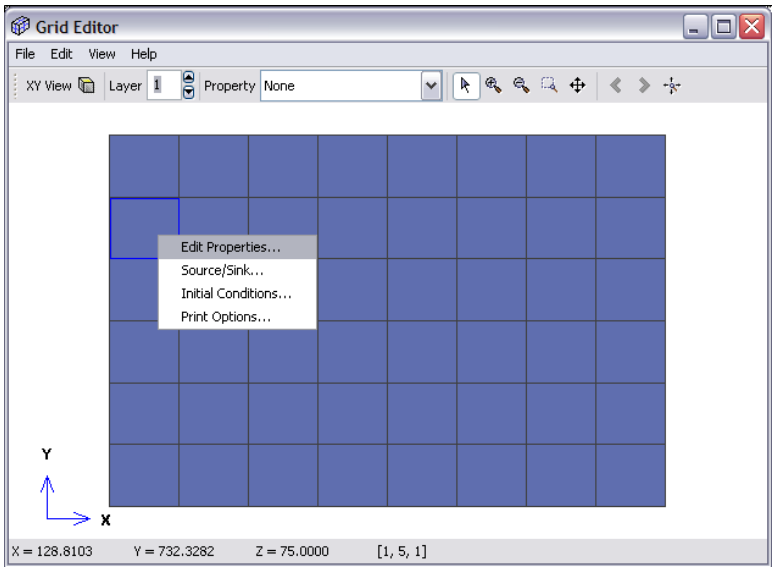

Figure 7.9. Editing a cell in the Grid Editor

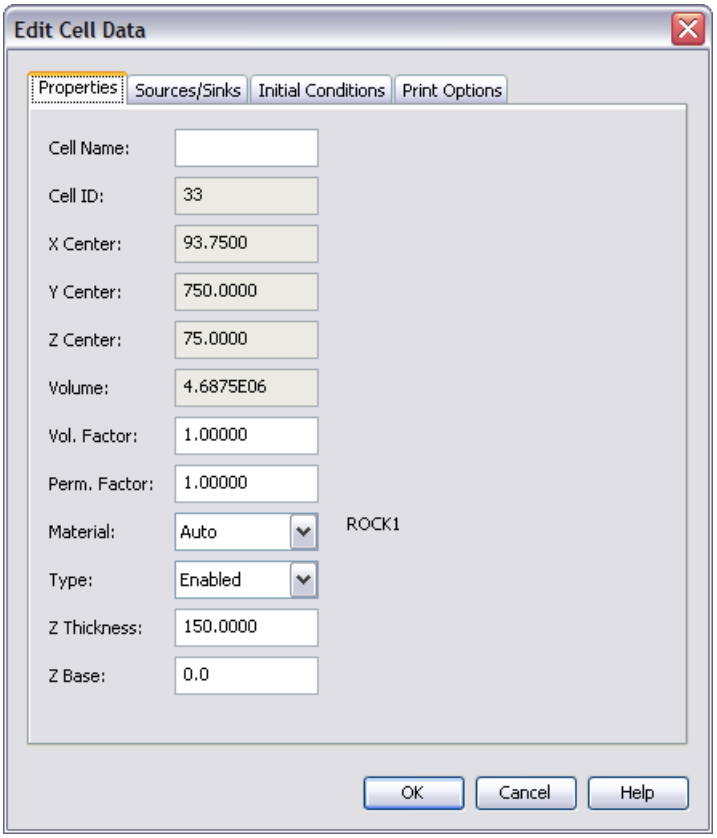

Figure 7.10. Editing cell properties

The Sources/Sinks and Initial Conditions tabs will be described in the Boundary Condition and Initial Condition chapters.

The Print Options tab is used to output cell data every time step for the selected cell (this is the FOFT file as used by TOUGH). In addition, connection data can be written (this is the COFT file as used by TOUGH).

Extra Cells

There are times when the capability to add non-geometric "extra" cells is useful. These extra cells can be used to define special boundary conditions or in other ways to "trick" the model into representing some special feature.

Support for "extra" cells is provided in PetraSim through dialogs. Since these cells are not geometric, the user must define the volume and connections of these cells to the regular grid cells. To create an extra cell, select **Model->Add Extra Cell...**. Figure 7.11 illustrates the definition of the basic cell properties. The user provides:

- Cell Name - A decriptive name that can be used to access cell results for plotting.

- Cell ID - This is calculated by PetraSim, not editable.
- Volume - The volume of the cell.
- Material - The material for the cell.
- Type - Enabled (included as standard cell), Disabled (not included in analysis), or Fixed State (set as fixed boundary condition). See PetraSim Basics for further details.

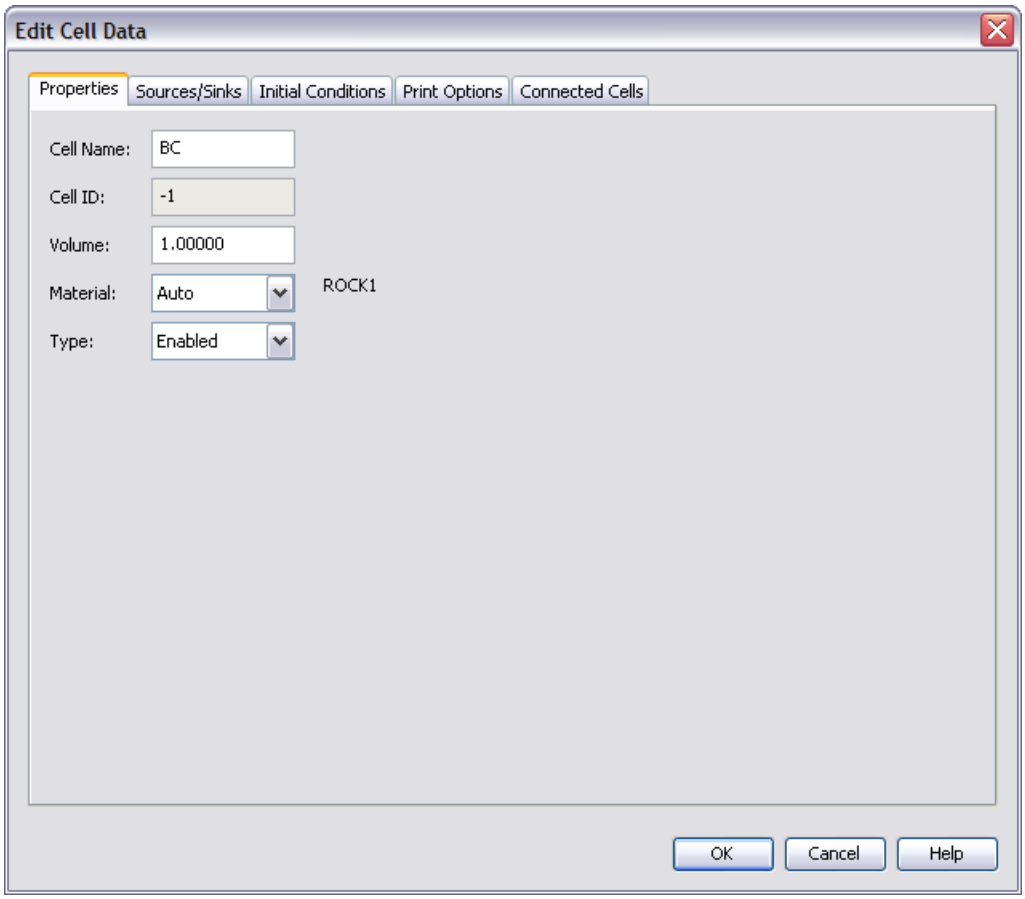

Figure 7.11. Defining the basic cell properties

The Sources/Sinks, Initial Conditions, and Print Options for an extra cell are the same as a standard cell.

The connections of the extra cell to the grid are specified by selecting the Connected Cells tab, Figure 7.12. The user must manually specify the connection data required by TOUGH. This includes:

- To Cell - This is the cell to which the extra cell is connected. This will be the cell ID of a cell in the mesh. You can find the cell ID of any cell using the Grid Editor

and then viewing the cell properties.

- Orientation - This is must be 1, 2, or 3 and corresponds to the PermX, PermY, or PermZ definitions in the material data.
- Dist. This - The distance of the connection in the extra cell. See TOUGH concepts "Spatial Discretization."
- Dist. To - The distance of the connection in the connecting cell.
- Area - The cross-sectional area of the connection.
- Gravitational Acceleration - The cosine of the angle between the graitational acceleration victor and the line between the two elements. If positive, the extra element is above the connecting "To" element.
- Radiative Heat Transfer - "Radian emmittance" factor for radiative heat transfer. Usually left as 0.0.

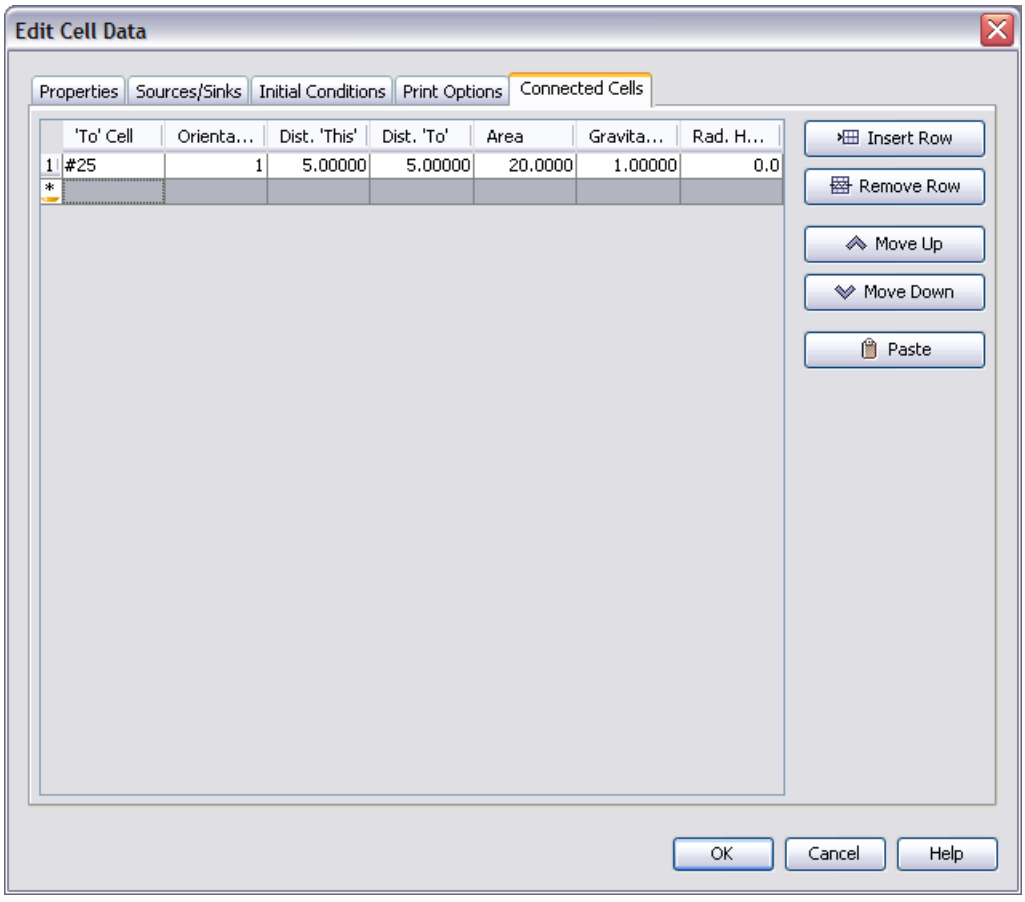

Figure 7.12. Defining the extra cell connections to the model

To edit an extra cell, double click on the extra cell in the Tree View.

Chapter 8. Materials

Material Data

Materials are used to define the permeabilities and other properties in an analysis. Each cell is associated with a material. Materials can be assigned to the entire model (when the boundary is created), by region (select a region and edit the region properties), or to individual cells (in the Grid Editor, select a cell or cells). PetraSim uses inheritance to determine any particular cell property: it first looks in the cell; if the property is not found there, it looks in the region; finally it looks in the default model.

When a new model is started, there is one default material. Material data is edited by selecting **Properties->Materials...** or . In this dialog, the user can edit, create, and delete materials, Figure 8.1. The basic material data includes (many are self-explanatory):

- Name - The material name that will be written to the TOUGH input file, limited to five characters.
- Description - A longer description for user clarity.
- Rock Density - Density.
- Porosity - Porosity
- X, Y, and Z Permeability - The absolute permeabilities are defined in each direction.
- Wet Heat Conductivity - Wet conductivity
- Specific Heat - Specific heat.

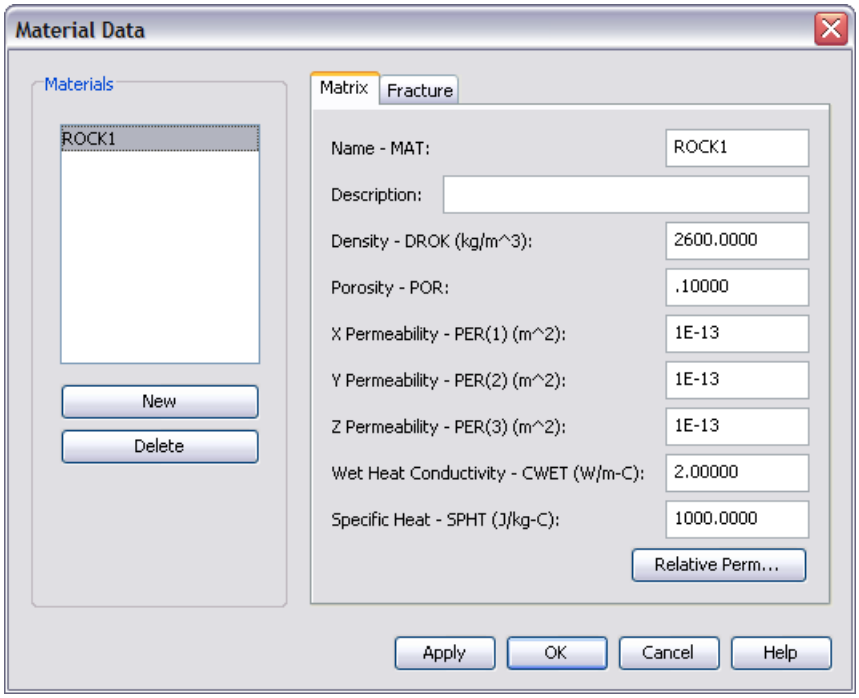

Figure 8.1. Material properties

Relative Permeability

Selecting the **Relative Perm...** button displays the Additional Material Data dialog. The first tab is used to define Relative Permeability, Figure 8.2. The user selects the desired relative permeability function and then defines the parameters used by that function. A graph will display the permeabilities (magenta->gas and blue->liquid) as a function of liquid saturation.

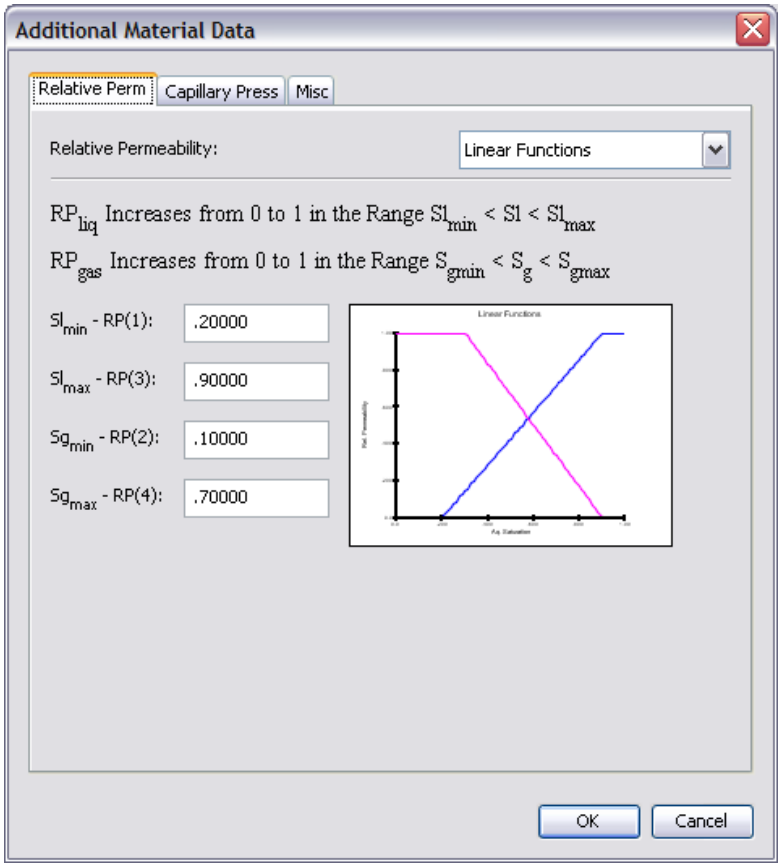

Figure 8.2. Relative permeability functions

Capillary Pressure

Select the Capillary Pressure tab to define the capillary pressure function, Figure 8.3. The user selects the desired capillary pressure function and then defines the parameters used by that function. The value of ICP corresponds to the TOUGH function ID. The Help section of www.petrasim.com provides a spreadsheet to plot the capillary pressure functions.

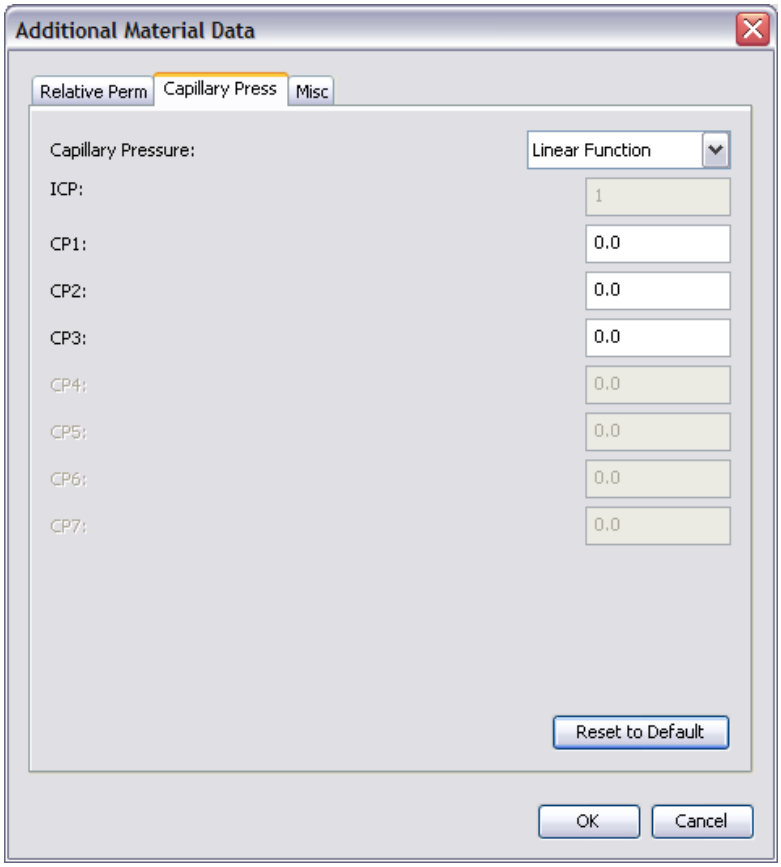

Figure 8.3. Capillary pressure functions

Miscellaneous Material Data

Select the Misc tab to define additional material properties, Figure 8.4. These include:

- Pore Compressibility - This defines how the pore volume changes as a function of pressure. This is used when storativity is to be included in the model, such as when performing a well test analysis. In most cases, this is not used and remains 0.0.
- Pore Expansivity - The defines how the pore volume changes with temperature. In most cases, this is not used and remains 0.0.
- Dry Heat Conductivity - Used with the wet heat conductivity to change the thermal conductivity of the rock.
- Tortuosity Factor - The user is referred to Appendix D of the TOUGH2 User's Guide for a detailed discussion of this factor. In most cases, this is not used and remains 0.0.
- Klinkenberg Parameter - The user is referred to Appendix A of the TOUGH2 User's Guide for a detailed discussion of this factor. In most cases, this is not used

and remains 0.0.

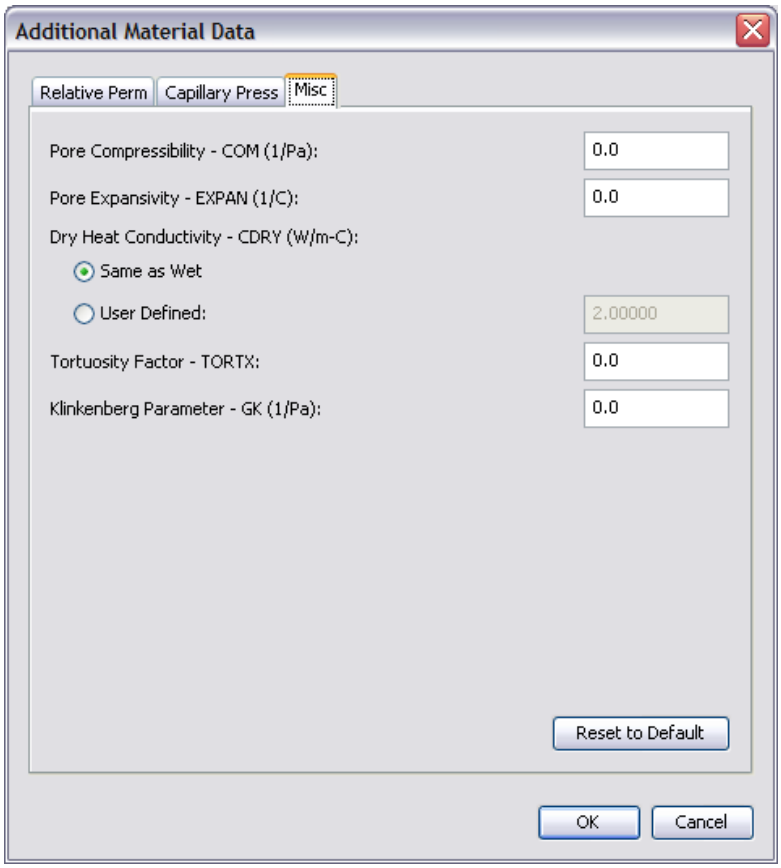

Figure 8.4. Miscellaneous material data

Assigning Different Materials by Cell

To support the use of geostatistical data, PetraSim allows the user to import a table of material assignments for all cells. This is useful if the user has an independent representation of the model that can be queried to obtain a spatial definition of materials. PetraSim provides two tools:

- The capability to write a file with cell IDs and X, Y, Z coordinates.
- The ability to paste a table of material types for all cells.

To write a file with cell IDs and X, Y, Z coordinates, select **File->Write Grid Data...**. This file defines the cell coordinates in their PetraSim order that allows you to query a separate material database.

Select **Model->Assign Cell Materials...** to open the Assign Cell Materials dialog, Figure 8.5. You can either type or paste a list of materials to be assigned to each cell. All materials must have already been defined. The Material Name must match the name of

an existing material.

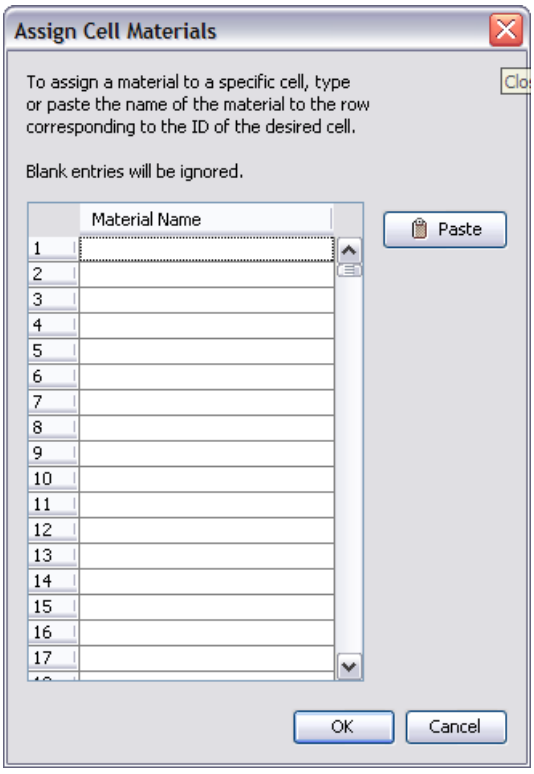

Figure 8.5. Assign Cell Materials dialog

Chapter 9. Initial Conditions

Initial conditions are used to define the initial state of each cell. A hierarchy is used to determine the cell state; if defined at the cell, those values are used; if defined at the region, those are used; finally, the default model initial conditions will be used.

The specific initial conditions are different for each EOS. For any specific EOS, there are at least single and two phase initial conditions, as well as options for different components. The user is referred to Chapter 3, Tough Concepts for a discussion of components and an example of setting single and two phase initial conditions.

Only for the simplest models will the initial conditions be uniform over the model. In most realistic analyses, a steady state simulation will be used to reach an equilibrium solution. For example, this will be used to reach gravity-capillary equilibrium in a vadose zone analysis or heat and fluid flow equilibrium in a geothermal reservoir analysis. The steady state results will then be used as initial conditions for the transient analysis. When this approach is used, two separate folders should be used to store the steady state analysis and the transient analysis.

Because of the complex physics represented in TOUGH, setting of the initial conditions can be challenging. The user is directed to the many examples available at the PetraSim web site for guidance on how others specify initial conditions.

Default Initial Conditions

Default initial conditions are always defined for the model. To set these conditions, select **Properties->Initial Conditions...** or to open the Default Initial Conditions dialog, Figure 9.1.

You will then be provided all the available initial condition options that are valid for the EOS and selected components. Based on your knowledge of the problem, define these appropriately.

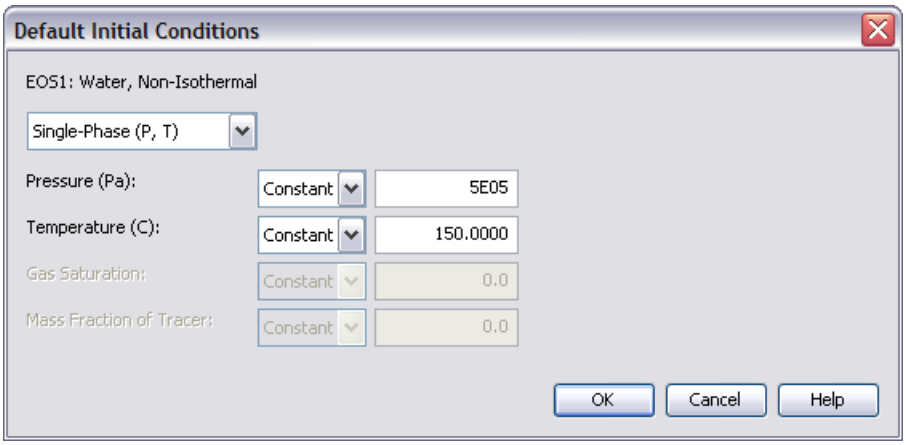

Figure 9.1. Setting default initial conditions

Region Initial Conditions

To define initial conditions by region of the model, select a region then select **Model->Edit Selection...**. On the Edit Region Data dialog, select the Initial Conditions tab. After selecting, Specify by Region, you will be able to define initial conditions for a region, Figure 9.2. If you do not want region initial conditions to be used, unselect Specify by Region.

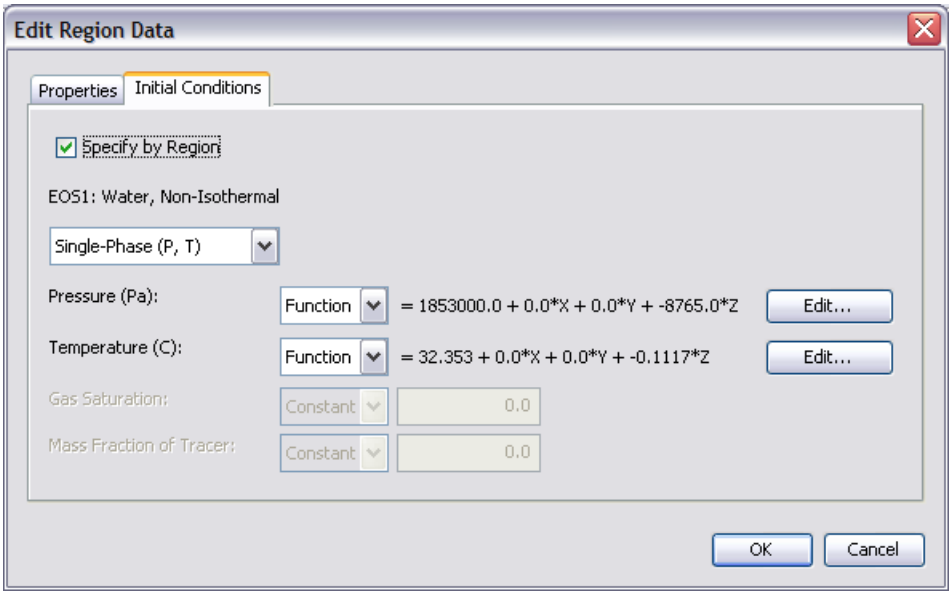

Figure 9.2. Setting region initial conditions

Cell Initial Conditions

To define initial conditions by cell, open the Grid Editor. Then right-click on a cell and select Initial Conditions in the context menu (or select a cell and **Edit->Properties...**. On the Initial Conditions tab of the Edit Cell Data dialog, select Specify Initial Conditions by Cell, Figure 9.3. You will then be able to define initial conditions for a cell. If you do not want cell initial conditions to be used, unselect Specify Initial Conditions by Cell.

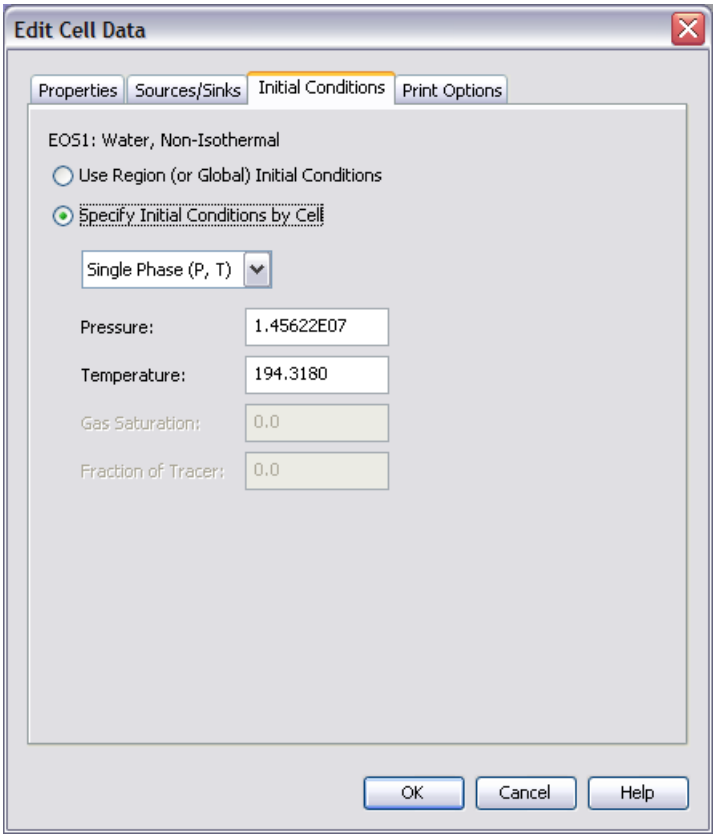

Figure 9.3. Setting cell initial conditions

Loading Previous Results as Initial Conditions

To read initial conditions from a previous analysis, select **File->Load Initial Conditions...** and read a previous SAVE file. The model used to write the SAVE file must have the same geometry as the model for which you are reading data. To avoid overwriting of files by TOUGH, each analysis should be run in a separate directory.

Recommended Examples

The TOUGH2 example problem 8 "Contamination of an Aquifer from VOC Vapors in the Vadose Zone" provides an excellent tutorial in the setting of two-phase capillary equilibrium initial conditions and the definition of an atmospheric boundary. A steady state analysis is used to define the initial conditions for the transient analysis.

The T2VOC Problem 2 example also demonstrates the use of a steady state analysis to define initial conditions, followed by several consecutive transient analyses representing a spill, spreading of the spill, and clean-up.

Chapter 10. Boundary Conditions

Fixed Boundary Conditions

Boundary conditions where the pressure, temperature and other variables do not change with time (called "essential" or Dirichlet boundary conditions) are typically set using "Fixed State" option in a cell. This is done by selecting the cell in the Grid Editor (see the chapter "The Solution Grid" for details).

A cell with fixed conditions will act as a source/sink for fluid and heat flow.

"Tricks" can be used to selectively fix the pressure or temperature independently. For example, to fix the pressure, the material of the cell can be changed so that the thermal conductivity is zero. Then, only fluid will flow to the cell and the cell will act as a fixed pressure. Similarly, the permeability could be set to zero for the cell to act as a fixed temperature condition.

Sources and Sinks

Sources and sinks are used to define flow into or out of the cell. These are typically used to define production from or injection into a cell. This is used for situations such as a well in a reservoir or rainfall on the surface.

The rates can be defined as constant or using a table to give time/rate pairs. By default, PetraSim assumes a step change when a time history of input is specified. This can be changed in the Solution Parameters options.

To define Sources/Sinks, open the Grid Editor and right-click on a cell to display the context menu. Select Sources/Sinks, Figure 10.1. The user now has several options:

- Heat - The rate of Heat In can be defined as a constant or though a table as a function of time. Use a negative number to remove heat.
- Mass Out - This defines the mass produced from the cell.
- Well on Deliverability - This defines a boundary condition where the cell produces to a fixed pressure. The user defines the Productivity Index and the pressure. See page 54 of the TOUGH2 User's Guide for instructions on calculation of the Productivity Index.
- Well from File - This is a coupled wellbore flow model. See page 66 of the TOUGH2 User's Guide for instructions on its use.
- Injection - Injection parameters will vary depending on the EOS being used. In general, the user will specify a rate and an enthalpy for each component to be injected.

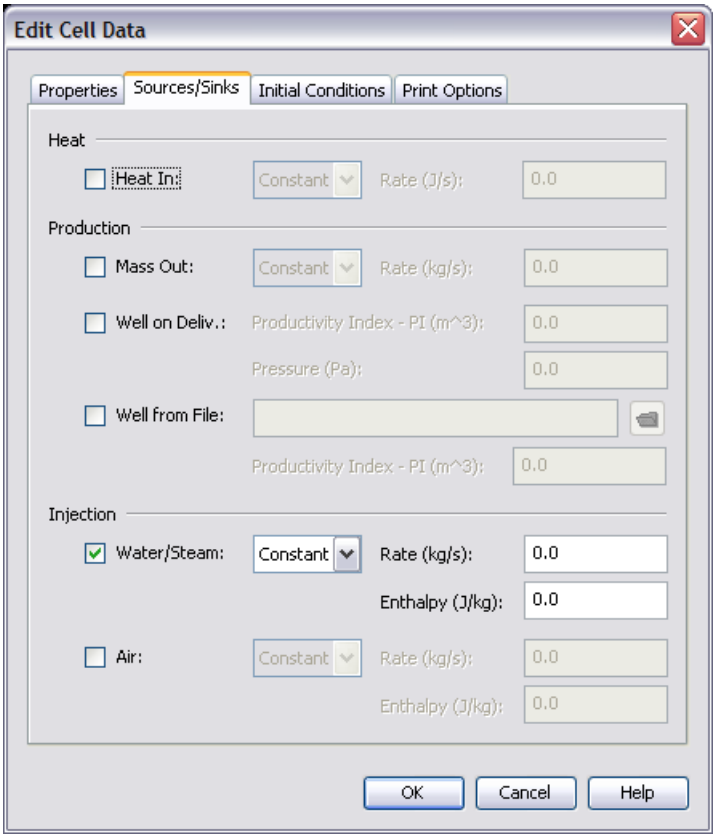

Figure 10.1. Editing cell properties

Using Wells in PetraSim

PetraSim provides a basic option to define wells as geometric objects (lines in 3D space). Injection or production options are assigned to the well and PetraSim handles the details of identifying the cells that are intersected by the well and applying the appropriate boundary conditions to each cell. This is not a true coupled well model, it is a means of identifying the cells that intersect a well and creating the individual sources/sinks for each cell. It also provides a way to label and display wells.

Adding a well and defining the boundary conditions is a two step process. Define the well coordinates by selecting **Add Well...** on the **Model** menu. Name the well and give the coordinates in order, either starting at the top or bottom of the well. The new well will be displayed in the tree view, double-click on the well to edit it; right-click to delete the well.

Once a well is created, you can define the minimum and maximum Z coordinates of the completion interval (the range over which the well can flow to the porous media). For models that will use the **Well on Deliverability** option, it is best if these completion bounds correspond to gridlines in the model. This is because the entire cell depth is used when calculating the **Well on Deliverability** flow. If the well will use the **k*h**

or **Uniform** options to distribute the flow, then the completion interval does not need to correspond to the gridlines.

Select the appropriate production or injection option. When flow rates are specified, the number is for the entire well. Flow into each cell the well intersects is apportioned either by k*h (permeability*height) or uniformly. If k*h is used, the total k*h is calculated for the entire well and then the flow into each cell is determined by the permeability and height (intersection length) for that cell. Using this approach, more flow is injected (produced) into cells with higher permeability. The uniform distribution proportions flow by the intersection length of each cell. In either of these cases, PetraSim creates individual sources/sinks for each cell intersected by the well. These sources/sinks are independent of each other.

For the **Well on Deliverability** option, the user can select the **Well Model** or **User Defined** gradient. The **Well Model** option activates the TOUGH2 well on deliverability model, where the pressure gradient is calculated using a depth dependent flowing density in the wellbore (see the TOUGH2 user manual). In this case, the specified pressure corresponds to the pressure at the center of the top cell in the well. If the **User Defined** gradient is selected, the pressure is that at the top of the completion interval and the user specifies the gradient directly. For both cases, follow the TOUGH2 guidelines for calculating the Productivity Index.

Time-Dependent Essential (Dirichlet) Boundary Conditions

Background

Although TOUGH2 provides an easy way to set constant essential (Dirichlet) boundary conditions using the "Inactive" cell option, there is no similar provision for time-dependent boundary conditions. There are two reasons for this decision:

- This places a significant burden on the user to ensure that all specified states would be physically meaningful.

- "The user could get into terrible problems when phase compositions change in the boundary cell, because then primary variables get switched. The user could end up interpolating between one number that means temperature, and another that means saturation [Pruess, 2003]."

The alternate approach is to inject or withdraw mass and/or heat from cells, thus accommodating any phase changes easily and naturally. That is, use natural (Neumann) boundary conditions to obtain the desired essential boundary conditions in the cell. However, since this is an indirect way to accomplish the desired goal, the user needs some guidance on how to accomplish this.

Setting the Time-Dependent Boundary Conditions

The boundary condition cells should be thought of as cells that are not part of the solution. Therefore, we can set material properties and other parameters in ways that are not tied to the actual problem to be solved. The following sections describe some use-

ful "tricks."

Use a Very Large Volume

The first concept is to make the volume of the cell with the boundary condition "very large" relative to the other cells in the grid. There is no absolute definition of "very large" but the concept is that the volume should be so large that flow in and out of the boundary condition cell to connected cells will have negligible effect on temperature or pressure in the boundary condition cell. A typical value could be a volume of 1.0E50 m3. In PetraSim, this can be accomplished by setting the volume multiplication factor to a large number (select a cell and then Edit Properties in the Grid Editor).

Setting a Temperature Condition

For a simple temperature boundary condition, we do not want flow into or out of the cell. This can be accomplished by making a special material that has zero permeability and small porosity and applying it to this cell. It is also necessary that the connections between the temperature boundary condition cells and the other cells in the model have a non-zero length in the boundary condition cell. The use of zero permeability and small porosity has two effects:

- Because of the small porosity, calculating the necessary heat input/output to change the cell temperature is easy, since there is negligible fluid in the cell and the rock specific heat can be assumed for the entire cell.

- Because of zero permeability, no fluid will flow from this cell into any connected cells (the non-zero length connections are also necessary). Note: Although zero permeability is the correct approach, the user should be aware that for upstream weighting of absolute permeability (MOP(11) = 0 or 1), it is still possible to force flow into a cell with zero permeability and non-zero nodal distance [Pruess, 2003].

We now set cell to the desired initial temperature and then specify the heat flow into (or out) of the cell to obtain the desired change in temperature.

This method is directly applicable in PetraSim.

Setting a Pressure Boundary Condition

Setting a pressure boundary condition can be accomplished in a similar manner as that used to set a temperature. In this case, a new material is created with zero thermal conductivity and assigned to the cell. As before, it is also necessary that the connections between the temperature boundary condition cells and the other cells in the model have a non-zero length in the boundary condition cell. The pressures in the cell can now be controlled by flow into and out of the cell (see the following example).

This method is directly applicable in PetraSim.

Caution: If the specified pressure results in flow from the boundary condition cell to connected cells, the heat transported by that flow will affect the temperature in the

connected cells.

Combined Pressure and Temperature Boundary Conditions for Single Phase Liquid

Experienced TOUGH2 users often apply simultaneous temperature and pressure boundary conditions by creating two boundary condition cells, as described above, and then connecting both boundary condition cells to the same cell in the model. TOUGH2 accommodates this, since it is not required that connections represent physically meaningful geometries. As noted, one danger with this approach is that the pressure boundary condition can lead to unwanted heat transport if the fluid flows from the boundary condition cell to connected cells. PetraSim supports this option through the use of "extra cells."

In the following we describe a way to accomplish the same objective, but using only physically meaningful geometry. This method also handles the combined pressure and temperature conditions in a way that usually corresponds to the desired physical behavior with respect to heat transport by flow out of the boundary condition cell.

Setting combined pressure and temperature boundary conditions will use the following concepts:

- A "very large" volume in the boundary condition cell. Consequently, "real" flow to connected cells in the model will have negligible change on either pressure or temperature in the boundary condition cell.

- A "somewhat larger" permeability in the boundary condition cell (maybe 1000 times the normal value). This means that fluid can flow into or out of the cell but that the pressure drop in the boundary condition cell will be approximately zero. Note: Pruess does not recommend changing the permeability due to possible numerical problems, but instead suggests changing the nodal distance to be small (1.0E-10). Since PetraSim uses true geometry, this approach can be approximated in PetraSim by using "thin" elements for the boundary cells.

- A "small" value for the porosity of the boundary condition cell. As a result, the rock heat capacity can be used to calculate the required heat flow to change temperatures.

- A "large" value of pore compressibility. This means that water compressibility can be neglected in the calculation of pressure changes due to flow into or out of the boundary condition cell and that changes in volume due to temperature changes will have negligible effect on pressure.

- Heat flow to the boundary condition cell will be specified to obtain the desired time-dependent boundary temperature.

- Water flow to the boundary condition cell will be specified to obtain the desired time-dependent boundary pressure.

Multi-Phase Pressure and Temperature Boundary Conditions

For multi-phase conditions, the pore compressibility can be left as zero, since the gas phase will serve the same purpose. The flow to control pressure would probably use the gas phase and would need to account for the mixture compressibility.

Solution Controls

The solution can not resolve transients to a level finer than the time step. Therefore, it is necessary to limit the maximum time step. For example, if the period of a transient is one day, it will be necessary to divide the day into several time steps (5 to 10) to capture the transient response.

By default, TOUGH2 averages the flow data at the beginning and end of the time step. This is fine if the transient is smooth and several time steps are used during to resolve the transient. If larger time steps are used, it is important to activate the rigorous step rate option (In PetraSim, Solution Controls/Options).

Example

The following example is based on a desire to specify time-dependent temperatures and pressures that represent the conditions for a stream in a groundwater calculation. The desired values are given in Figure 10.2 and Figure 10.3.

Days	Time (sec)	Temperature (C)	Pressure (Pa)
0	0	19.16	105409.8525
1	86400	18.64	110401.2634
2	172800	19.55	116677.8879
3	259200	19.52	116229.5576
4	345600	18.89	111297.9241
5	432000	17.94	109414.9367
6	518400	17.25	113001.5793
7	604800	17.70	115841.0046
8	691200	17.53	112015.2526
9	777600	17.68	108936.7177
10	864000	17.53	107621.6154
11	950400	17.30	106904.2869
12	1036800	16.66	106426.0679
13	1123200	15.90	106067.4037
14	1209600	15.33	106515.734
15	1296000	14.90	120653.0834
16	1382400	14.90	115512.2291
17	1468800	14.77	114346.5702
18	1555200	14.88	112702.6924
19	1641600	15.21	110102.3765
20	1728000	15.04	108906.829

Figure 10.2. Desired boundary conditions

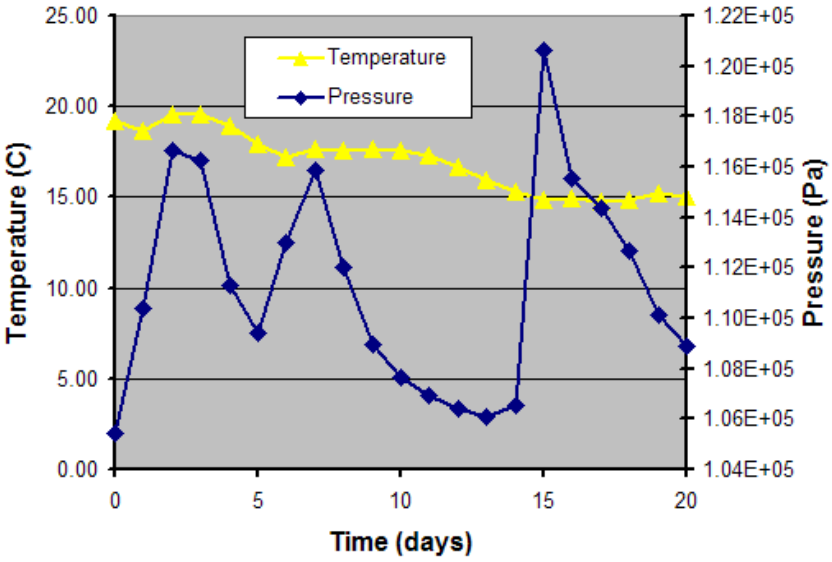

Figure 10.3. Graph of desired boundary conditions

For the example, create a cell with dimensions of 1 m on each side, but set the volume factor to be 1.0E50. We set the material properties as Figure 10.4.

Property	Value
Rock Density (kg/m3)	2600
Rock Porosity	0.001
Permeability (m2)	1E-13
Specific Heat (J/kg-C)	1000
Pore Compressibility (1/Pa)	1.-E-6

Figure 10.4. Desired boundary conditions

We calculate the heat flux as follows:

$$\dot{Q} = V\rho c_p \frac{\Delta T}{\Delta t}$$

where $\dot{Q}$ is the heat flux, V is the cell volume, ρ is the rock density, c_p is the rock heat capacity, ΔT is the change in temperature, and Δt is the change in time. Note that since the porosity is very small, we only use the rock properties and apply this to the entire cell volume. The calculated values are shown in Figure 10.5.

Time (sec)	Temperature (C)	Heat Flux J/s
0	19.16	-1.56481E+51
86400	18.64	2.73843E+51
172800	19.55	-8.85769E+49
259200	19.52	-1.89335E+51
345600	18.89	-2.86741E+51
432000	17.94	-2.066E+51
518400	17.25	1.35346E+51
604800	17.70	-5.2337E+50
691200	17.53	4.58592E+50
777600	17.68	-4.55279E+50
864000	17.53	-6.77021E+50
950400	17.30	-1.92931E+51
1036800	16.66	-2.28261E+51
1123200	15.90	-1.72943E+51
1209600	15.33	-1.29663E+51
1296000	14.90	8.85926E+48
1382400	14.90	-4.0093E+50
1468800	14.77	3.328E+50
1555200	14.88	1.00634E+51
1641600	15.21	-5.15039E+50
1728000	15.04	6.36209E+48
	15.00	

Figure 10.5. Desired boundary conditions

Similarly, we calculate the required fluid flow rates using:

$$\dot{m} = \rho_{water}\,\phi V C\,\frac{\Delta P}{\Delta t}$$

where: ρ_{water} is the density of water, ϕ is the porosity, C is the pore compressibility, and ΔP is the change in pressure. The calculated values are shown in Figure 10.6.

Time (sec)	Pressure (Pa)	Flow kg/s
0	105409.8525	5.77132E+42
86400	110401.2634	7.25735E+42
172800	116677.8879	-5.18382E+41
259200	116229.5576	-5.7022E+42
345600	111297.9241	-2.1772E+42
432000	109414.9367	4.14706E+42
518400	113001.5793	3.28309E+42
604800	115841.0046	-4.42353E+42
691200	112015.2526	-3.55956E+42
777600	108936.7177	-1.52059E+42
864000	107621.6154	-8.29411E+41
950400	106904.2869	-5.52941E+41
1036800	106426.0679	-4.14706E+41
1123200	106067.4037	5.18382E+41
1209600	106515.734	1.63463E+43
1296000	120653.0834	-5.94411E+42
1382400	115512.2291	-1.34779E+42
1468800	114346.5702	-1.90073E+42
1555200	112702.6924	-3.00662E+42
1641600	110102.3765	-1.38235E+42
1728000	108906.829	0
	108906.829	

Figure 10.6. Desired boundary conditions

These are input to TOUGH2. Note that this is a bit tricky, since injection and production must both be set on the same cell. This means that two separate conditions must be set. The injection for flow in and the production for flow out. Set these terms zero when the other is acting, that is, during injection, the production is zero and during production the injection is zero.

The resulting plots show excellent agreement between temperatures, and not quite as good agreement for pressures.

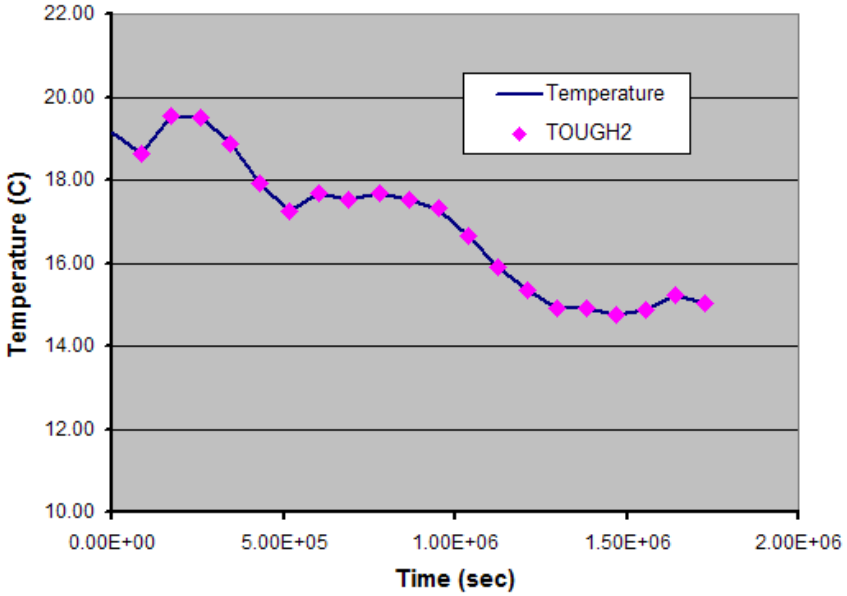

Figure 10.7. Comparison of desired and calculated boundary condition temperatures

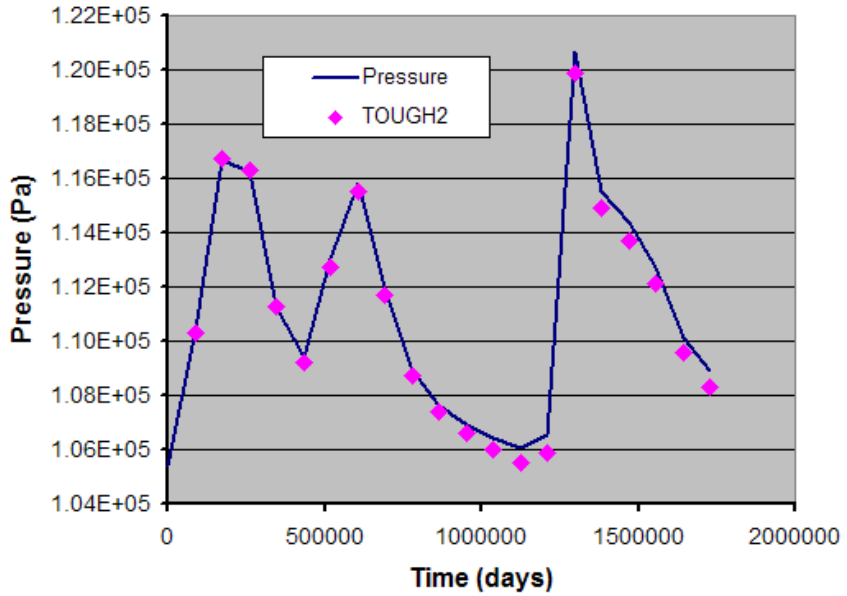

Figure 10.8. Comparison of desired and calculated boundary condition pressures in TOUGH2

Chapter 11. Solution and Output Controls

Solution Controls

The Solution Controls dialog allows the user to specify all aspects that will be used by TOUGH in solving the problem. To set these controls, select **Analysis->Solution Controls...** or to open the Solution Controls dialog.

Times Tab

Select the Times tab, Figure 11.1. This dialog is used to input all data related to solution times and time step control.

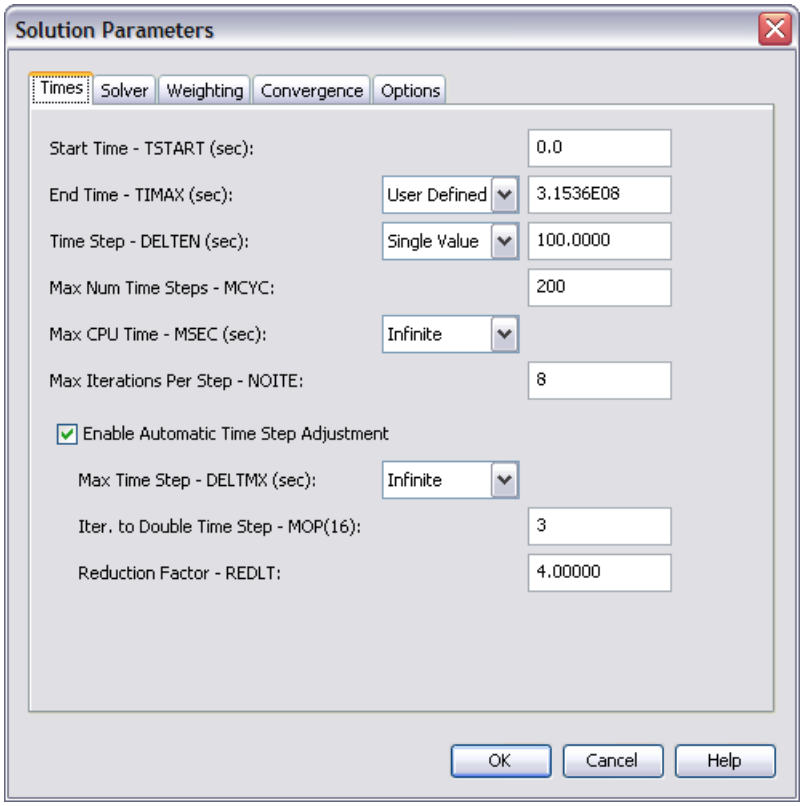

Figure 11.1. The Times tab controls

- Start Time - The start of the analysis. In most cases this will be 0.0.
- End Time - The end time of the analysis. Usually specified, but can be set to infinite and then solution will run for the Max Num Time Steps
- Time Step - User control of the time steps. If Automatic Time Step Adjustment is enabled (recommended), this is the initial time step used in the analysis. The user

can also specify a table of time steps for the solution. If a list of time steps is given, the last time step will be used until the End Time is reached. If the user has selected to define the time steps in a table and enabled Automatic Time Step Adjustment, the specified table of time steps is used first, with automatic adjustment after if the number of solution time steps exceeds the number of time steps in the list.

- Max Num Time Steps - The maximum number of time steps for the solution. If this number is exceeded, the analysis ends.
- Max CPU Time - A control to limit the maximum CPU time used in the analysis. If this number is exceeded, the analysis ends
- Max Iterations per Step - The maximum number of iterations for a time step. If exceeded and Automatic Time Step Adjustment is enabled, then time step will be reduced.
- Automatic Time Step Adjustment - If selected, the time step size will be automatically adjusted (recommended).
- Max Time Step - Maximum time step that will be used when adjusting the time step.
- Iter. to Double Time Step - If convergence is reached in this number of iterations, then time step size will be increased.
- Reduction Factor - If convergence fails in Max Iterations per Step, then time step will be reduced by this factor.

Solver Tab

Select the Solver tab, Figure 11.2. TOUGH provides conjugate gradient and direct solvers, with several options. The user can select the solution method and options for that method. Either the Preconditioned Bi-Conjugate Gradient (default) or Stabilized Bi-Conjugate Gradient methods are recommended.

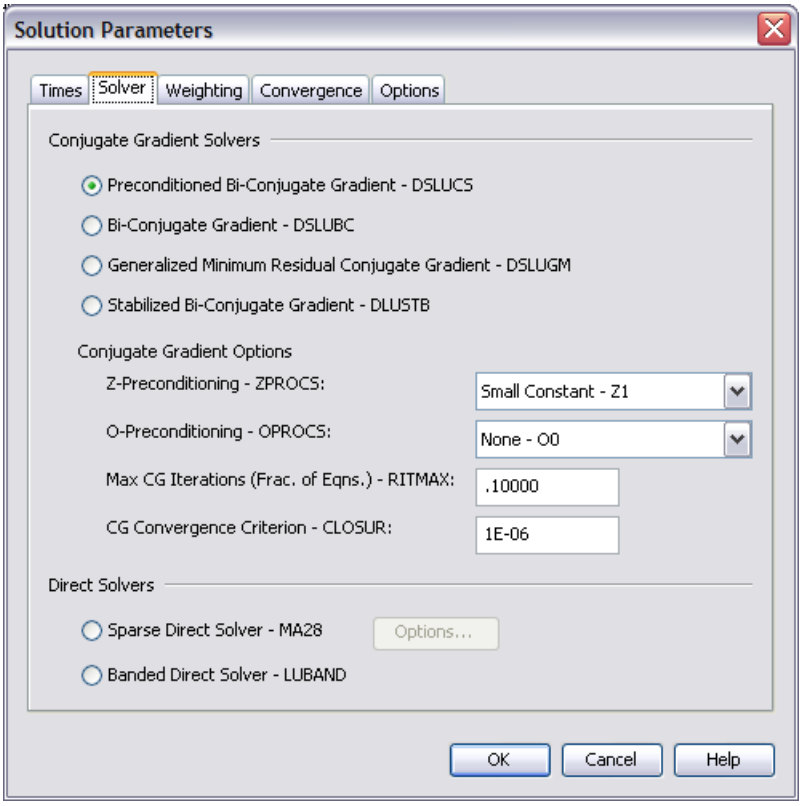

Figure 11.2. The Times tab controls

Weighting Tab

Select the Weighting tab, Figure 11.3. These are advanced TOUGH2 options. For most users, the default values are appropriate. See the TOUGH2 manual for more detailed descriptions.

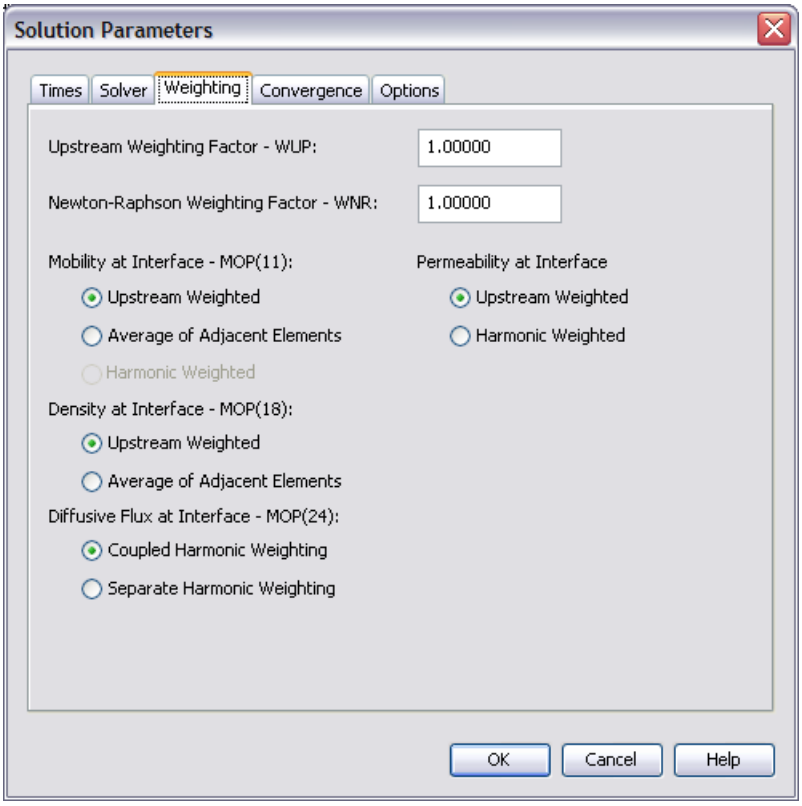

Figure 11.3. The Times tab controls

Convergence Tab

Select the Convergence tab, Figure 11.4. Advanced convergence options. In most cases, the user will not change these parameters.

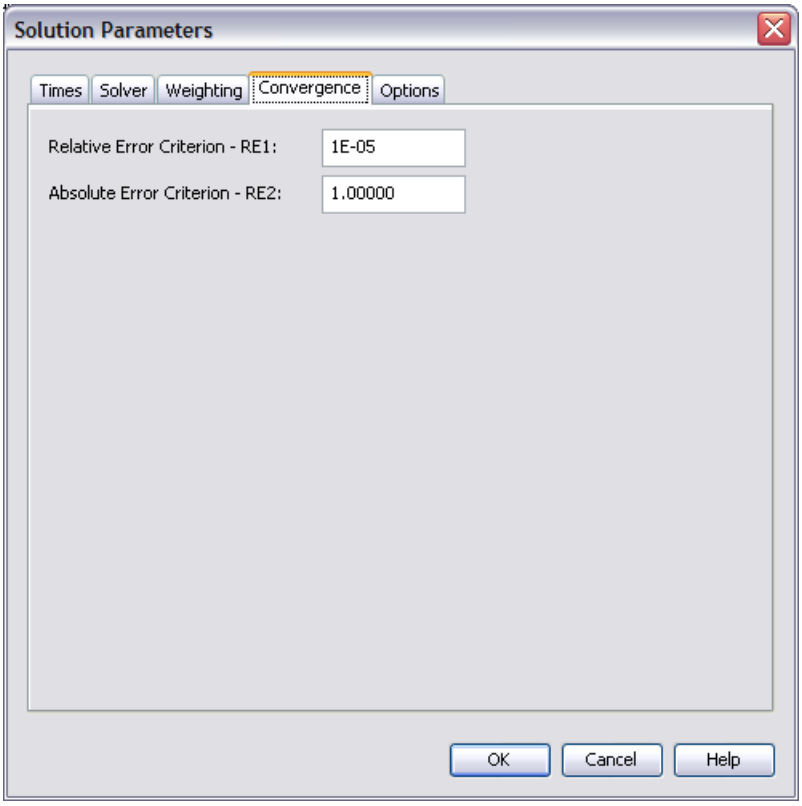

Figure 11.4. The Times tab controls

Options Tab

Select the Options tab, Figure 11.5. Advance options. In most cases, these will not be changed by the user.

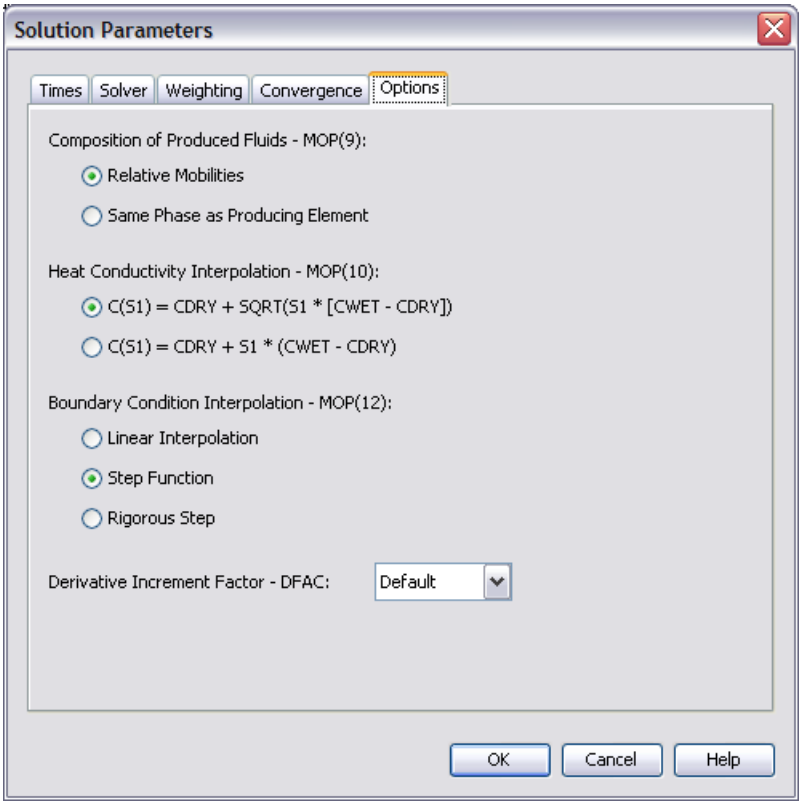

Figure 11.5. The Times tab controls

Output Controls

The Output Controls dialog allows the user to specify output options. To set these controls, select **Analysis->Output Controls...** or to open the Output Controls dialog, Figure 11.6.

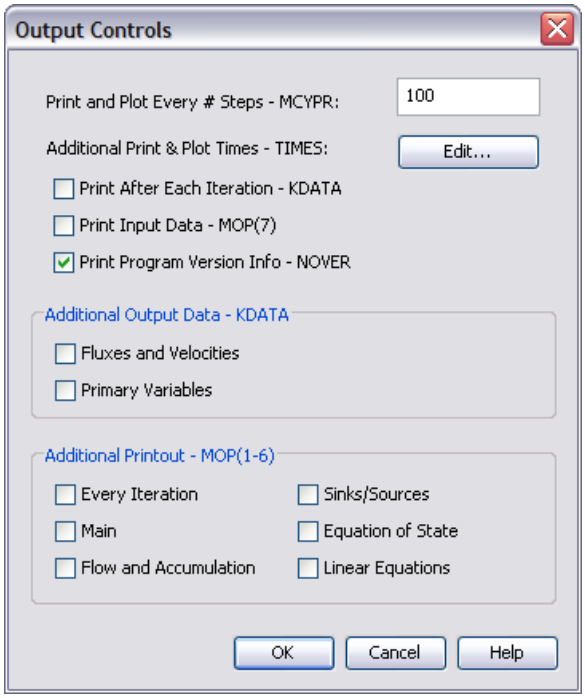

Figure 11.6. Output controls dialog

Output Controls options include:

- Print and Plot Every # Steps - Output will be written at the specified time step increment.
- Additional Print and Plot Times - This opens a table in which you can give specific times at which output is desired.
- Additional Output Data - Select fluxes and velocities to have the output data necessary to include flux arrows in the 3D plots. Selecting Primary Variables is usually only used for debugging purposes.
- Additional Prinout - These options are usually only used for debugging purposes.

Chapter 12. Running Simulation

Running a Simulation

Except for TOUGH-Fx/HYDRATES, all the TOUGH executables are included as an integral part of the PetraSim software. To execute the appropriate TOUGH module, on the **Analysis** menu, click **Run TOUGH2** or click . This will first save the PetraSim model file and then the TOUGH2 Simulation Run dialog will be displayed, Figure 12.1.

The Running TOUGH2 dialog displays simulation time steps on the X-axis and the log10 of the time step on the Y-axis. As a rule of thumb, an increasing Y value is a good sign of simulation progress. If your time steps start to become smaller, it may indicate that the simulator is having a difficult time converging.

When the simulation finishes, a message will be displayed and the Cancel button will turn into a Close button. Click the **Close** button.

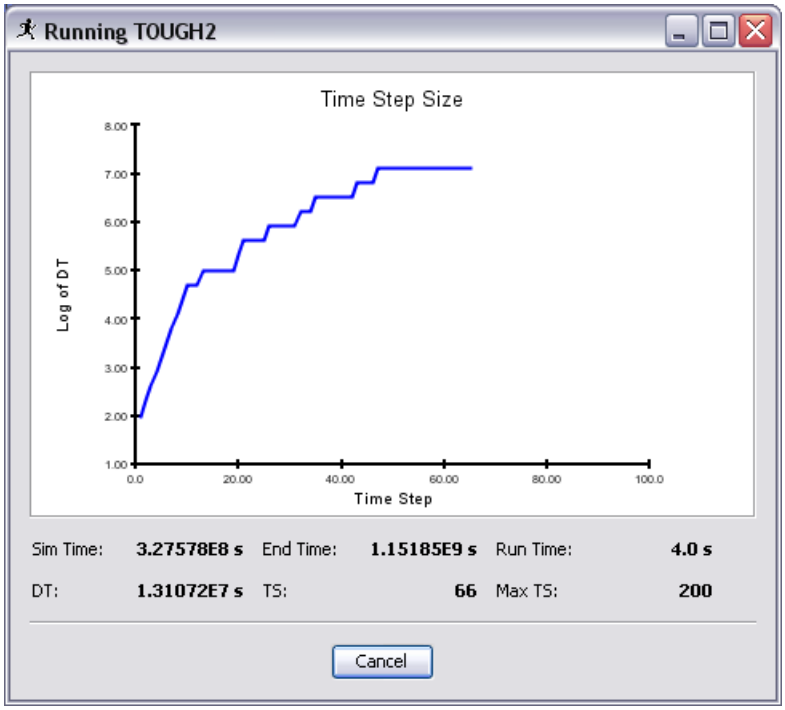

Figure 12.1. Running the TOUGH analysis

Setting TOUGH Analysis Priority

A TOUGH analysis makes heavy demands of the computer processor; if you are running a single core computer, you may want to reduce the priority of the TOUGH analysis. Start the Task Manager (Cntrl+Alt+Delete or right-click on the lower toolbar). On the Processes tab, click on CPU to sort by the process using the most CPU (you

many need to click twice to bring highest CPU users to the top of the list). You will see a process such as "EOS7.exe". Right-click on the process, select Set Priority and select Low. Close the dialog.

Setting the priority low will keep your computer response snappy to other tasks and allow the CPU to support the TOUGH analysis when not needed for other tasks.

Monitoring Progress of TOUGH Analysis

During the TOUGH analysis, there are several ways to monitor progress. One way is to go to the problem directory and, using a text editor, open the *.out file as it is written by TOUGH. In this file will be text similar to the following:

```
 ****************************************************
    260(  21,  3) ST = 0.209715E+09 DT = 0.104858E+09
    365(  22,  3) ST = 0.419430E+09 DT = 0.209715E+09
     51(  23,  4) ST = 0.838861E+09 DT = 0.419430E+09
    216(  24,  4) ST = 0.125829E+10 DT = 0.419430E+09
    258(  25,  4) ST = 0.167772E+10 DT = 0.419430E+09
```

The first number is the ID of the cell with the smallest time step. The first number in the parantheses is the time step counter and the second number is the number of iterations required for that step to converge. ST is the total solution time. DT is the solution time increment.

Writing the TOUGH Input File

Most users will not need to explicitly save a TOUGH input file, since this is automatically written when the analysis is performed. However, if you are using TOUGH-Fx/HYDRATE or if you have a special TOUGH executable, you can select **File->Wrute TOUGH2 File...** to write the standard TOUGH input file. This file can then be edited (if necessary) and used to run your special TOUGH executable from the commmand line. Save the output to filename.out (where filename is the name of the PetraSim file) and you can then read the results for plotting in PetraSim.

Chapter 13. Plotting Results

PetraSim reads the TOUGH output files to make plots of results. The user can make 3D or time history plots of the data. When a plot is displayed, selecting **File/Export Data...** will allow the user to export the current plot data in either Tecplot or spreadsheet format.

3D Plots of Results

To make a 3D plot of results, select **Results->3D Results...** or . This will open a new window with a display of the model and pressure isosurfaces at the first output time, Figure 13.1.

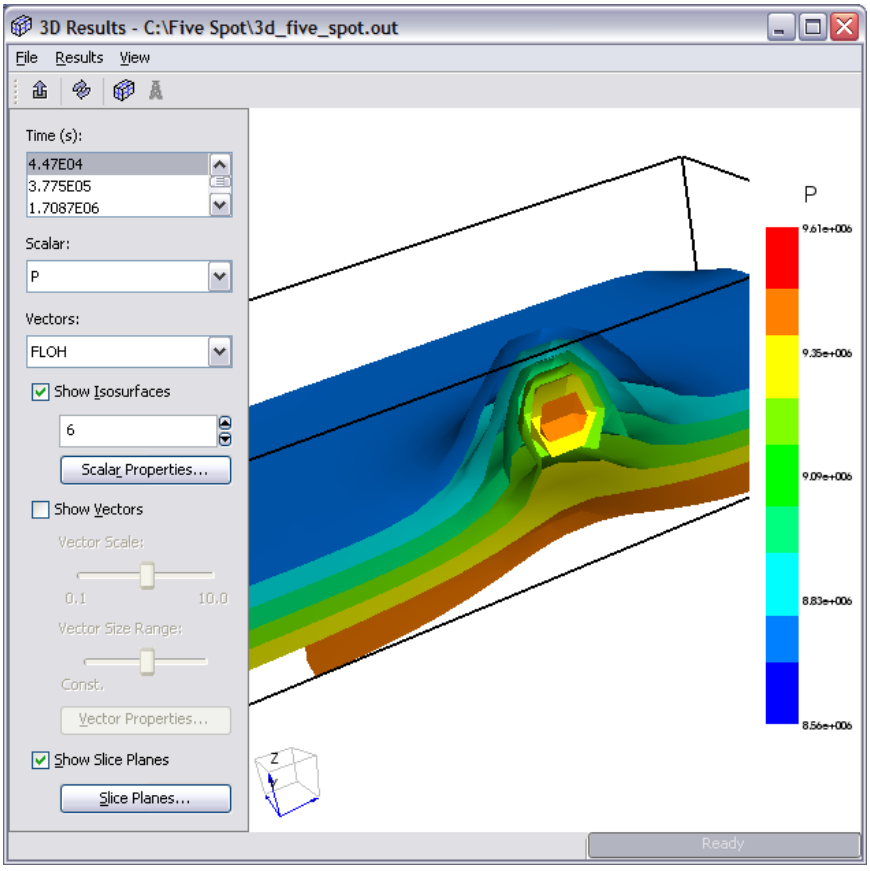

Figure 13.1. The 3D results window

Plot controls include:

- Time (s) - A window that displays all the available output times. Select one of these times for plotting.
- Scalar - Select the output parameter for plotting. The scalar parameter is the one

that will be used for isosurfaces and contours on slice planes. The list of parameters is dynamically created from the TOUGH output file and will be different for each EOS.

- Vectors - If vector data was written to the output (this must be selected as one of the Output Controls options), this will display a list of available vector data. The list of parameters is dynamically created from the TOUGH output file and will be different for each EOS.

- Show Isosurfaces - This checkbox turns on the display of isosurfaces for the selected scalar. The number indicates how many isosurfaces will divide the plot range. Selecting the **Scalar Properties...** button displays a dialog, Figure 13.2, on which you can specify a specific plot range, choose to use a logarithmic scale, and specify the number of colors used on contour plots.

- Show Vectors - If vector information is available, selecting the checkbox will turn on the display of vector data, Figure 13.3. The Vector Scale, controls the scaling factor applied to the vectors and the Vector Size Range controls the relative size of the longest to shortest vectors. By default, both the relative size and color of the vectors correspond to the magnitude of the vector. Moving the Vector Size Range to the left will result in all vectors having the same length. Selecting the **Vector Properties...** button displays a dialog, Figure 13.4, in which the user can set the range for vectors and choose whether the vector color should indicate the magnitude.

- Show Slice Planes - Turns on slice planes on which contours of the scalar parameter are displayed. Select the **Slice Planes...** button to define the axes normal to the planes and the coordinates of the planes, Figure 13.5. Typical plots are shown in Figure 13.6

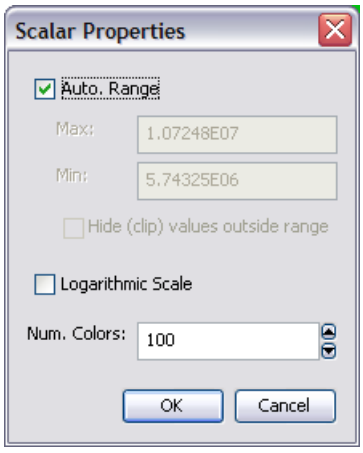

Figure 13.2. Scalar Properties dialog

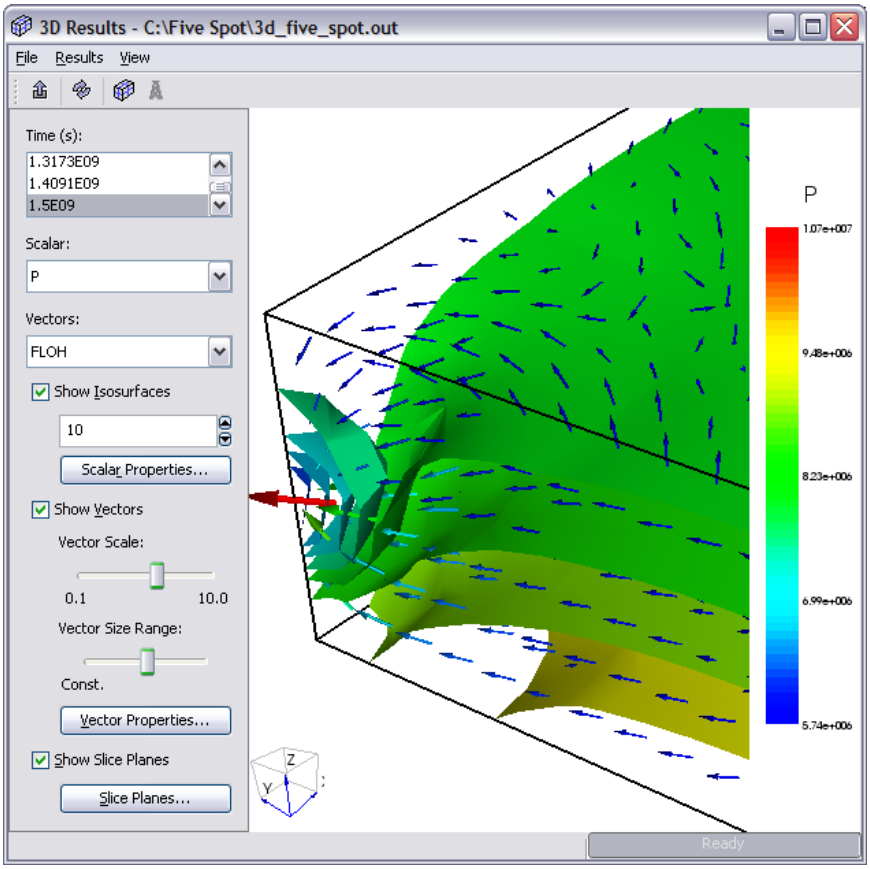

Figure 13.3. The 3D results window

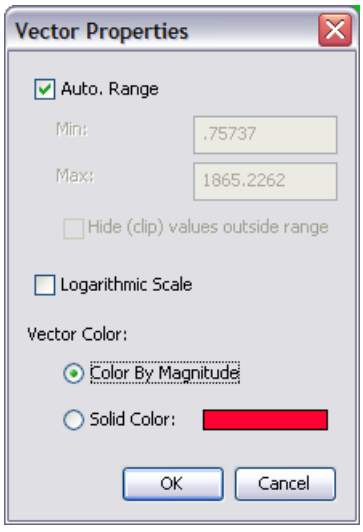

Figure 13.4. Vector Properties dialog

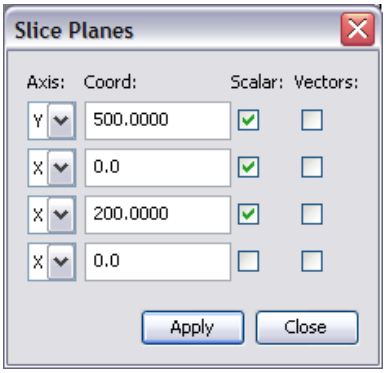

Figure 13.5. Slice Planes dialog

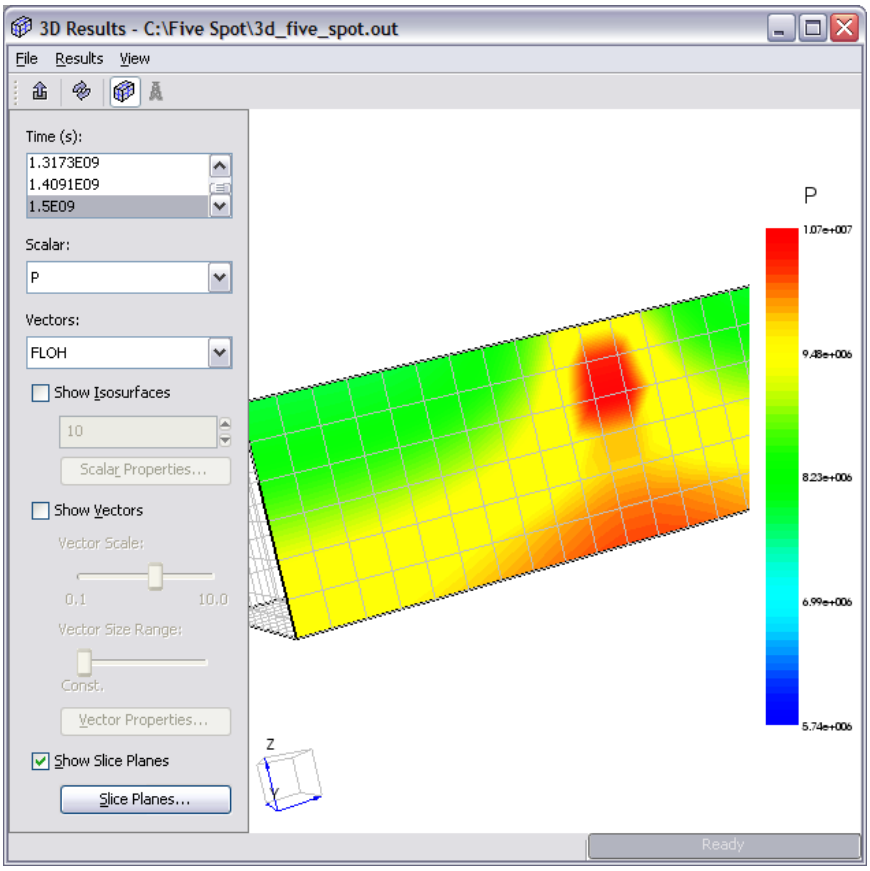

Figure 13.6. Example of contours on slice planes

Select **File->Export Data...** to write a file that can be read into Tecplot. The format of the data will be a value and then the X, Y, and Z coordinates. The data can be written either at the center or corners of each cell.

Time History Plots of Results

To make a time history plot, select **Results->Cell History Plots...** or . This will open a new window, Figure 13.7.

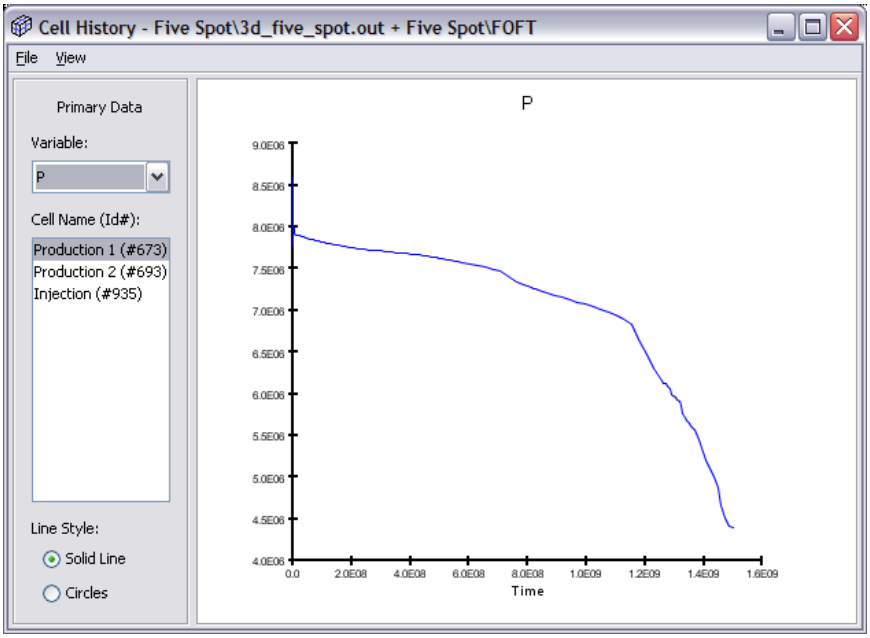

Figure 13.7. Example of contours on slice planes

You can select the Variable to plot and the Cell Name of the cell. The Cell Name is the name given in the Grid Editor to that cell. Time history plotting for a cell is also activated in the Grid Editor.

By default, only the cells for which time history data have been requested or which have been given a name are listed. However, you can select **View->All Cells** to expand the list to all cells. When all cells are selected, data will only be available at the times in the standard output file. For cells for which time history output was specified, the results are available at each time step.

Source/Sink and Cell History Plots

This section explains the flow plots created by PetraSim and how to obtain time histories of cells that have sources/sinks.

The model used as an example represents production from a highly permeable layer at about 500m depth (average P = 5 MPa, constant T = 25 ºC, single-phase conditions). The model uses EOS1 and extends for 500x500x20m with a grid of 10x10x4 cells. An initial hydrostatic solution was run. In the production run, two of the boundaries are set to a fixed state and cell 169 uses a “Well on Deliverability” condition with a Productivity Index of 6.0E-9 and a Pressure of 5.0E6 Pa.

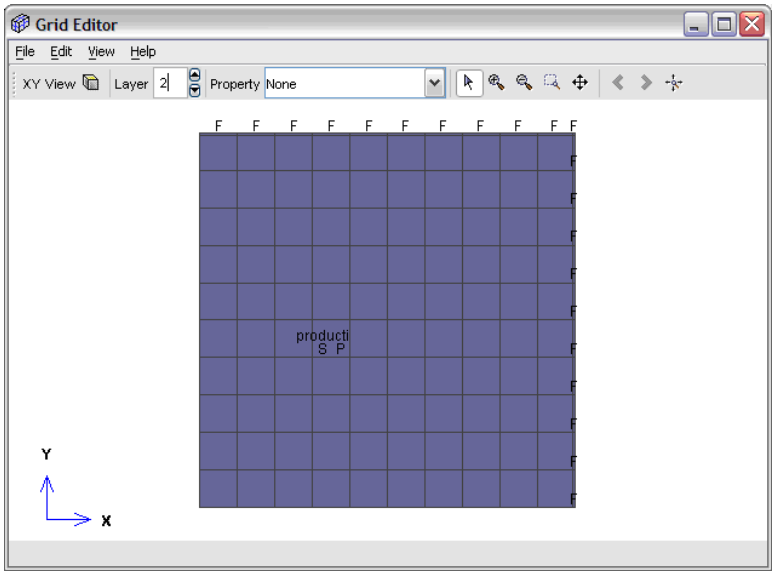

Figure 13.8. Production cell in layer 2 of example problem

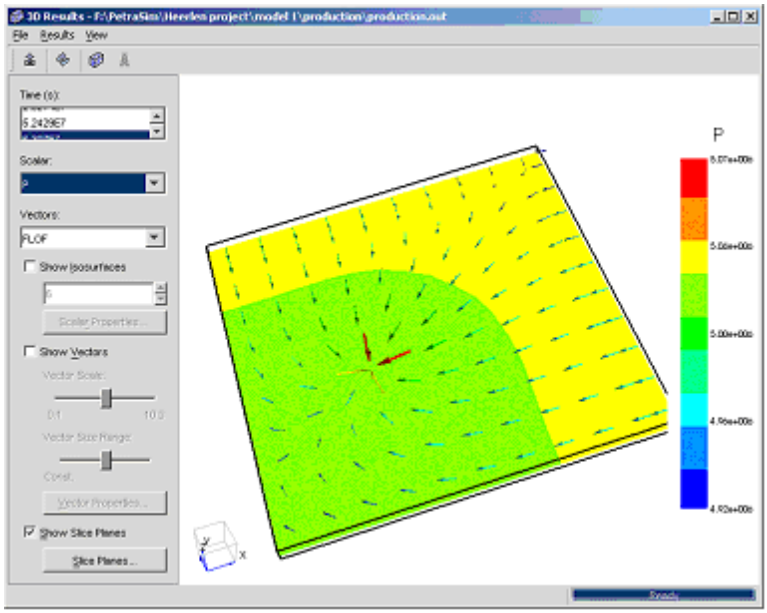

Figure 13.9. Plot of production flow

Probably the most important piece of information for a source/sink is the flow rate into/out of the cell. This can be plotted by selecting **Results->Source/Sink Plots...**, Figure 13.10. To make this plot, the Y Scale Range was adjusted to Min Y = -135.2, Max Y = 0.0 (use **View->Range...**V). This plot indicates that the production rate is 135.0 kg/sec. The user can export the plot.

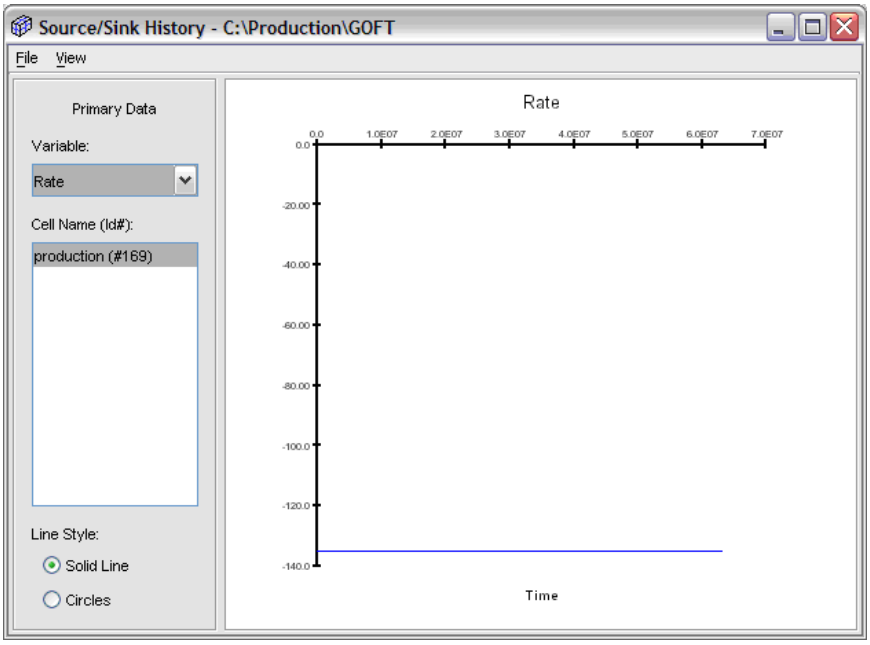

Figure 13.10. Plot of production from cell 169

The user can also obtain this information by looking at the TOUGH2 output file. At the end of every printed time step, the source/sink data is given, as shown below. This data shows that the generation rate is -135.0 kg/s, which matches the PetraSim plot.

```
TOUGH2 Analysis

KCYC =   20  -  ITER =    1  -  TIME = 0.63070E+08

ELEM SRC INDEX    GENERATION RATE    ENTHALPY    X1         X2
                    (KG/S) OR (W)     (J/KG)

169  1   1         -0.13500E+03     0.10940E+06  0.10E+01  0.00E+00
```

To understand the cell history flow plots it is necessary to know the cell names and connections. Figure 13.11 shows the cells names and how they are physically connected for the cells adjacent to cell 169. The production cell is 169 and it is connected to adjacent cells in layer 2 and to cell 48 in layer 1 and cell 290 in layer 3.

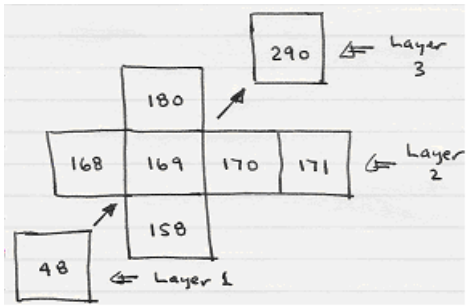

Figure 13.11. Connections for cell 169

We will first focus on the flow plot for cell 170, since that is the simplest. The user can select **Results->Cell History Plots...**, then select **View->All Cells...**, and select FLOF(X) for cell #170 to see the to see the plot shown in Figure 13.12. Select **File->Export Data...** to view the numerical value of -0.029 kg/s-m2.

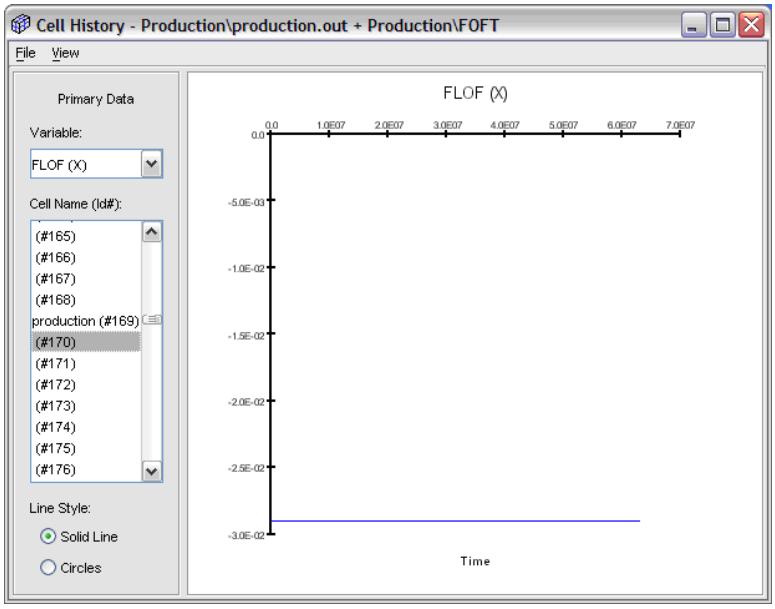

Figure 13.12. Plot of FLOF(X) for cell 170

The flow data plotted in the Cell History plot is the flux averaged at that cell. If we go to the output file, we can obtain the actual values of flow for each connection. A part of the file is shown below.

```
EL1   EL2   INDEX     FLOH        FLOH/FLOF        FLOF     FLO(GAS)      FLO(AQ.)   FLO(WTR2)
                        (W)          (J/KG)         (KG/S)    (KG/S)        (KG/S)     (KG/S)

169   170   385 0.107373E+07 0.109403E+06 0.981440E+01 0.000E+00 0.981440E+01 0.000E+00
170   171   386 0.513309E+06 0.109404E+06 0.469187E+01 0.000E+00 0.469187E+01 0.000E+00
171   172   387 0.340934E+06 0.109404E+06 0.311627E+01 0.000E+00 0.311627E+01 0.000E+00
172   173   388 0.268545E+06 0.109405E+06 0.245460E+01 0.000E+00 0.245460E+01 0.000E+00
```

```
173   174   389 0.233448E+06 0.109405E+06 0.213379E+01 0.000E+00 0.213379E+01 0.000E+00
```

For the connection between cells 169 and 170, the flow is 9.81 kg/sec. For the connection between cell 170 and 171, the flow is 4.69 kg/sec. To calculate the average X flux at cell 170, we average the two flows and divide by the area between the cells (250m2 since the cell face width is 50m and the cell height is 5m). The resulting value is 0.029 kg/s-m2, which matches Figure 13.10.

In the plot the negative sign indicates that the X flux is in the negative X direction. This is consistent with the positive connection sign convention used by TOUGH2. For a connection between cell 1 and cell 2, a negative FLOF indicates a flow from cell 1 to cell 2. A positive FLOF indicates flow from cell 2 to cell 1.

We now look at the more complex case of flow into cell 169, which is a production cell. The user can select **Results->Cell History Plots...** and select FLOF(X) to see the plot shown in Figure 13.13. This is a graph of fluid flux in the X direction at cell 169. The value is -0.00368 kg/s-m2, which value can be displayed by selecting **File->Export Data...**.

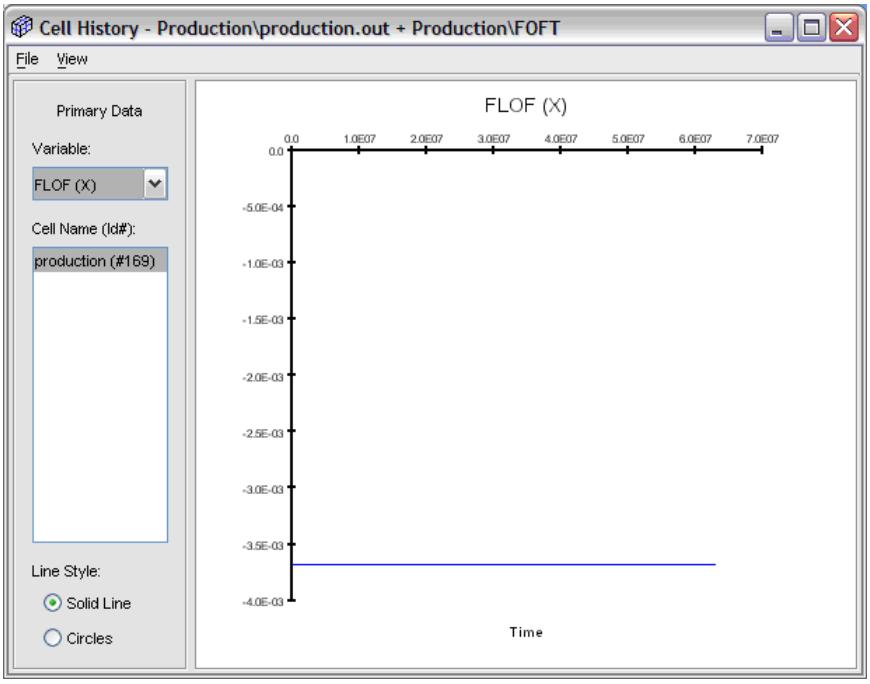

Figure 13.13. FLOF(X) plot for cell 169

If we look in the output file, we will find the following data for the connections, Figure 13.14.

Connection	FLOF
168->169	-7.97
169->170	9.81
158->169	-7.95
160->180	9.95
48->169	-34.32
169->290	64.98

Figure 13.14. Data for connections to cell 169

Using these values and the sign convention for flows, the flows into cell 169 are represented in Figure 13.15.

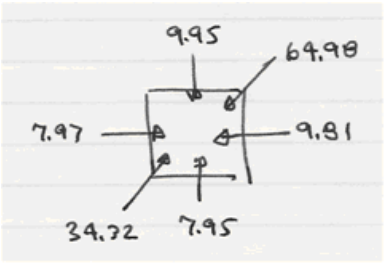

Figure 13.15. Flows into cell 169

If we sum these flows, the total is 135.0 kg/sec, consistent with previously discussed source/sink data.

This also illustrates why the flux data for a source/sink cell is not very useful. Since this cell is a production cell, there is flow in from the left and in from the right. The average X flux is then ((7.97-9.81)/2)/250 = -0.00368 kg/s-m2, which matches Figure 13.13.

Thanks to Hildenbrand Alexandra for providing this model.

Chapter 14. Flow in Fractured Media

The MINC Approach

TOUGH uses the "Multiple INteracting Continua" (MINC) method to approximate modeling fluid and heat flow in fracture-porous media. As described in [Pruess, 1992], "The method is applicable to flow processes in which an important aspect is the exchange of fluid, heat, or chemical species between fractures and unfractured rock. ... MINC can only be applied to media in which the fractures are sufficiently well connected so that a continuum treatment of flow in the fracture network can be made." If the fractures are not sufficiently connected, a discrete representation of the fracture should be used with a different porous material for flow in the fracture. A detailed explanation of MINC is provided in [Pruess, 1983].

As described in [Pruess, 1992], "The method is an extension of the double-porosity concept, originally developed by [Barenblatt, et al., 1960] and [Warren and Root, 1963]. It is based on the notion that fractures have large permeability and small porosity (when averaged over a reservoir subdomain), while the intact rock (the rock "matrix") has the opposite characteristics. Therefore, any disturbance in reservoir conditions will travel rapidly through the network of interconnected fractures, while invading the matrix blocks only slowly."

MINC is implemented in TOUGH as a mesh processor of the mesh. Additional cells and connections are created so that matrix blocks are "discretized into a sequence of nested volume elements which are defined on the basis of distance from the fractures. Continuum #1 represents the fractures, continuum #2 represents matrix rock in close proximity to the fractures, continuum #3 represents matrix rock at larger distance, etc. In response to an imposed disturbance in the fracture system, fluid and/or heat can migrate in the matrix blocks outward towards the fractures, or inward away from the fractures.

For a complete description, the user is referred to [Pruess, 1992] and [Pruess, 1992], copies of which are available in the help section of http://www.petrasim.com.

Using MINC in PetraSim

To activate the MINC option in PetraSim, select **Properties->Global Properties...** or . Go to the MINC tab, Figure 14.1. Select "Enable Multiple Interacting Continua (MINC)". Then, the input data corresponds to that given in the TOUGH2 User's Guide,.

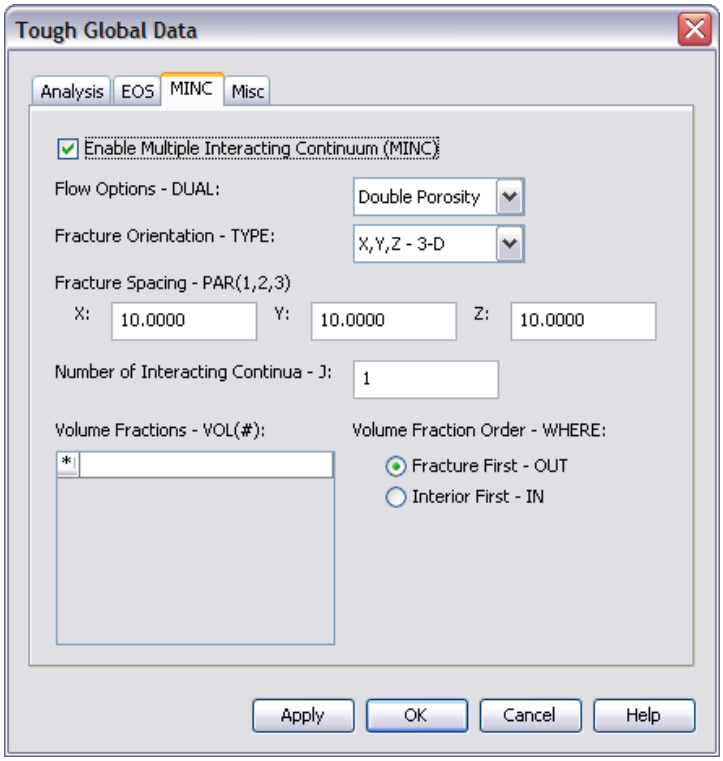

Figure 14.1. Activating MINC in PetraSim

Once the MINC option is activated, the user will need to specify the fracture material data on the Fracture tab of the Material Data dialog. This will be the data used for the fractures. The Matrix data will be used for the rock matrix.

Chapter 15. Miscellaneous

Map Between TOUGH2 Names and PetraSim Interface

For experienced TOUGH2 users, this map provides a listing of where TOUGH2 constants are defined in PetraSim. Italics are used to indicate a menu item. The map is organized following the TOUGH2 User's Guide format. In addition, one each dialog, the TOUGH name for each input variable is provided.

TITLE

- TITLE - *Properties->Global Properties* in Tough Global Data dialog on Analysis tab.

MESHM

This is only used with the MINC option. MINC data is given in *Properties->Global Properties* in the Tough Global Data dialog on the MINC tab.

ROCKS

ROCKS.1 Record

- MAT - *Properties->Materials* in Material Data dialog.
- NAD - Automatically determined based on user input.
- DROK - *Properties->Materials* in Material Data dialog.
- POR - *Properties->Materials* in Material Data dialog.
- PER(I) - *Properties->Materials* in Material Data dialog.
- CWET - *Properties->Materials* in Material Data dialog.
- SPHT - *Properties->Materials* in Material Data dialog.

ROCKS.1.1 Record

- COM - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- EXPAN - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- CDRY - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.
- TORTX - *Properties->Materials* Select **Relative Perm...** button in Material Data

dialog. On Misc tab Additional Material Data dialog.

- GK - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog.

- XKD3 - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for EOS7R.

- XKD4 - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for EOS7R.

- FOC - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Misc tab Additional Material Data dialog. Only shown for T2VOC.

ROCKS.1.2 Record

- IRP - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. Automatically determined from selection on Relative Perm tab of Additional Material Data dialog.

- RP(I) - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Relative Perm tab of Additional Material Data dialog.

ROCKS.1.3 Record

- ICP - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. Automatically determined from selection on Capillary Press tab of Additional Material Data dialog.

- CP(I) - *Properties->Materials* Select **Relative Perm...** button in Material Data dialog. On Capillary Press tab of Additional Material Data dialog.

ROCKS.2 Record

- Automatically written.

MULTI

Automatically written based on EOS type and EOS options selected on *Properties->Global Properties* in Tough Global Data dialog on EOS tab.

START Record

Automatically written.

CHEMP (T2VOC only)

Automatically written for T2VOC based on VOC data specified in *Properties->Global Properties* in Tough Global Data dialog on EOS tab.

PARAM

PARAM.1 Record

- NOITE - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- KDATA - Automatically determined from selections on*Properties->Output Controls* in the Print and Plot Options dialog.
- MCYC - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- MSEC - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- MCYPR - *Properties->Output Controls* in the Print and Plot Options dialog.
- MOP(1) through MOP(7) - Automatically determined from selections on *Properties->Output Controls* in the Print and Plot Options dialog.
- MOP(9) - *Properties->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(10) - *Properties->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(11) - *Properties->Solution Controls* in Solution Parameters dialog on Weighting tab.
- MOP(12) - *Properties->Solution Controls* in Solution Parameters dialog on Options tab.
- MOP(13) - Not implemented. Used only by T2DM option.
- MOP(14) - *Properties->Solution Controls* in Solution Parameters dialog on Solver tab.
- MOP(15) - *Properties->Boundary Conditions* in Boundary Conditions dialog.
- MOP(16) - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- MOP(17) - *Properties->Solution Controls* in Solution Parameters dialog on Solver tab.
- MOP(18) - *Properties->Solution Controls* in Solution Parameters dialog on Weighting tab.
- MOP(19) - *Properties->Global Properties* in Tough Global Data dialog on EOS

tab, as appropriate.

- MOP(20) - Not implemented. Used only by EOS4 option.
- MOP(21) - Not used. Instead the alternate SOLVR record is used to select the solver. Select the solver in *Properties->Solution Controls* in Solution Parameters dialog on Solver tab.
- MOP(22) - Not implemented. Used only by T2DM option.
- MOP(23) - Not implemented. Used only by T2DM option.
- MOP(24) - *Properties->Solution Controls* in Solution Parameters dialog on Weighting tab.
- TEXP - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Select Molecular Diffusion and specify on Edit Coefficients dialog. For T2VOC on EOS tab.
- BE - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Select Molecular Diffusion and specify on Edit Coefficients dialog.
- DIFF0 - *Properties->Global Properties* in Tough Global Data dialog on EOS tab. Only for T2VOC.

PARAM.2 Record

- TSTART - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- TIMAX - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- DELTEN - Automatically determined based on options selected in *Properties->Solution Controls* in Solution Parameters dialog on Times tab. You can edit the table of time steps.
- DELTMX - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- ELST - Not implemented, instead select cell for printing in Grid Editor.
- GF - *Properties->Global Properties* in Tough Global Data dialog on Misc tab.
- REDLT - *Properties->Solution Controls* in Solution Parameters dialog on Times tab.
- SCALE - *Properties->Global Properties* in Tough Global Data dialog on Misc tab.

PARAM.2.1, 2.2, etc. Record

- Automatically written if table is used to give time steps in *Properties->Solution Controls* in Solution Parameters dialog on Times tab.

PARAM.3 Record

- RE1 - *Properties->Solution Controls* in Solution Parameters dialog on Convergence tab.
- RE2 - *Properties->Solution Controls* in Solution Parameters dialog on Convergence tab.
- U - *Properties->Solution Controls* in Solution Parameters dialog on Solver tab.
- WUP - *Properties->Solution Controls* in Solution Parameters dialog on Weighting tab.
- WNR - *Properties->Solution Controls* in Solution Parameters dialog on Weighting tab.
- DFAC - *Properties->Solution Controls* in Solution Parameters dialog on Options tab.

PARAM.4 Record

- This record is not used. Instead, initial conditions for each element are written using the INCON record, see below.

INDOM

This record is not used. Instead, initial conditions for each element are written using the INCON record, see below.

INCON

These records are created for each element based on initial condition data. The appropriate data is EOS dependent. See the Initial Conditions chapter for help with defining initial conditions.

SOLVR

This record is written based on options selected in *Properties->Solution Controls* in the Solution Parameters dialog on the Solver tab.

FOFT

The FOFT record defines a list of cells for which output data will be written to a file every time step. This record is written automatically by PetraSim, based on the cells that have been selected for detailed printing.

To select a cell for output, open the Grid Editor and right-click on a cell. Go to the Print Options tab. Use the check box to turn on printing. In the Properties tab, you can give the cell a name that will be displayed in the plot. After the analysis is completed and a time history plot made, the data can be written to a file for import into a spreadsheet.

GOFT

Automatically written for all sources and sinks.

NOVER

NOVERsion Record

- *Properties->Output Controls* in Output Controls dialog.

DIFFU

DIFFUsion Record

- All diffusion data is input from *Properties->Global Properties* in the Tough Global Data dialog on the EOS tab. Select Molecular Diffusion and then the Edit Coefficients button and dialog. Not valid for T2VOC.

SELEC

SELECtion Record

- Automatically written from data input on *Properties->Global Properties* in the Tough Global Data dialog on the EOS tab.

RPCAP

This record is not used. Instead, all data is written as part of ROCKS record.

TIMES

TIMES Record

- A table of output times can be specified in *Analysis->Output Controls* in the Output Controls dialog. These times are then written to the TIMES record.

ELEME

All element (cell) data is written based on the grid defined by the user.

CONNE

All connection data is written based on the grid defined by the user.

GENER

The GENER record defines a list of cells with source or sink boundary conditions. See Boundary Conditions chapter.

Chapter 16. Troubleshooting

Convergence Problems

It is inevitable that some of the analyses you run will stop execution before your specified end time. Usually this is because of convergence problems during the solution.

To determine what is the cause of the problem, you will need to open the TOUGH output file and learn to read it. Identifying why the model stops running is probably not going to be simple. Models that run for a while and then stop are the hardest to debug. TOUGH2 can get into frustrating convergence problems. TOUGH2 is a pretty good code, but the physics are complex, so if the problem gets into an unrealistic condition, it will stop. Tracking down the cause of a convergence problem may not be trivial.

Following is the step-by-step process used to look at one user's convergence problems. The user was learning about PetraSim and TOUGH2, so was developing the skills needed to run analyses.

STEP 1: Open the *.out file and looked for the messages printed before the data for the last time step. This will be before the text "THE TIME IS", so you can search for that text. A sample is copied below. DT is the time step and you can see that it has gotten very small -- 0.0488 sec. We also see that it can not find the parameters for element 11126 and the problem is that the TEMPERATURE is out of range in SAT. The TEMPERATURE value is 0.999, so it looks like something is cooling down to freezing and TOUGH2 can not handle that (the new TOUGH-FX version can handle freezing). Jump to step 2.

```
QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 144,  1]
TEMPERATURE = 0.999981E+00  OUT OF RANGE IN SAT
+++++++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
+++++++++   XX(M) = 0.118536E+06 0.549628E+00 0.999981E+00
+++++++++ REDUCE TIME STEP AT ( 144,  1) ++++++  NEW DELT = 0.488281E-01

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 144,  1]
11126( 144,  1) ST = 0.176848E+05 DT = 0.488281E-01 DX1= 0.000000E+00 ...

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 145,  1]
TEMPERATURE = 0.999996E+00  OUT OF RANGE IN SAT
+++++++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
+++++++++   XX(M) = 0.118536E+06 0.549627E+00 0.999996E+00
+++++++++ REDUCE TIME STEP AT ( 145,  1) +++++   NEW DELT = 0.244141E-01

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 145,  1]
11126( 145,  1) ST = 0.176848E+05 DT = 0.244141E-01 DX1= 0.000000E+00 ...

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 146,  1]
11126( 146,  1) ST = 0.176849E+05 DT = 0.488281E-01 DX1= 0.000000E+00 ...

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 147,  1]
TEMPERATURE = 0.999996E+00  OUT OF RANGE IN SAT
+++++   CANNOT FIND PARAMETERS AT ELEMENT *11126* IND = 4
+++++   XX(M) = 0.118536E+06 0.549627E+00 0.999996E+00

+++++ CONVERGENCE FAILURE ON TIME STEP # 147 WITH DT = 0.976562E-01 SECONDS,
     FOLLOWING TWO STEPS THAT CONVERGED ON ITER = 1
     STOP EXECUTION AFTER NEXT TIME STEP
+++++ REDUCE TIME STEP AT ( 147,  1) ++++++++++   NEW DELT = 0.244141E-01

QQQQQQQQQQ SUBROUTINE QU QQQQQQQQQQQQQQQQQQQQ --- [KCYC,ITER] = [ 147,  1]
11126( 147,  1) ST = 0.176849E+05 DT = 0.244141E-01 DX1= 0.000000E+00 ...
```

```
TOUGH2 Analysis

OUTPUT DATA AFTER ( 147,  1)-2-TIME STEPS    THE TIME IS  0.20469E+00 DAYS
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

TOTAL TIME     KCYC   ITER  ITERC   KON
0.17685E+05    147       1    689     2
   DX1M        DX2M        DX3M        DX4M        DX5M        DX6M
0.00000E+00 0.00000E+00 0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


ELEM.  INDEX     P           T           SG          SW        SO
               (PA)      (DEG-C)

   1    1 0.42499E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
   2    2 0.42344E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
   3    3 0.42299E+06 0.20003E+02 0.00000E+00 0.10000E+01 0.00000E+00
```

STEP 2. Go to the bottom of the *.out file and do an upward search for 11126 with the intent of finding out the current state of that cell. However, the first hit is at the source/sink output and is listed below. So knowing that cell 11126 is a source/sink with a generation rate, the first guess is that the generation rate is larger than can be supported by the flow into the cell and as a result pressure and temperature are dropping in that cell. Go to step 3.

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

        TOUGH2 Analysis

        KCYC =  147  -  ITER =    1  -  TIME = 0.17685E+05

ELEMENT SOURCE INDEX TYPE GENERATION RATE  ENTHALPY    FF(GAS)     FF(AQ)
                        (MOLE/S) OR (W)  (J/MOLE)

11126       1    1  COM1   0.22003E+03  0.00000E+00
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
```

STEP 3: Continue the search for 11126 to get the state of the cell until we find the P, T, etc data, as given below (the last line is for cell 11126). This confirms that the temperature is dropping. The saturation of gas is also lower in this cell. So now let us go and look at the cell in more detail. Go to step 4.

```
ELEM.  INDEX     P           T           SG          SW        SO
               (PA)      (DEG-C)

111 4 8995 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 5 8996 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 6 8997 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 7 8998 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 8 8999 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
111 9 9000 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11110 9001 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11111 9002 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11112 9003 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11113 9004 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11114 9005 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11115 9006 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11116 9007 0.10102E+06 0.19999E+02 0.87874E+00 0.12126E+00 0.00000E+00
11125 9008 0.10102E+06 0.19987E+02 0.87838E+00 0.12162E+00 0.00000E+00
11126 9009 0.11854E+06 0.10000E+01 0.45037E+00 0.54963E+00 0.00000E+00
```

STEP 4: Now we need to find the cell in the model. Cells are numbered in X,Y, Z order starting at the bottom layer. This example model has 36 cells in the X directly and 39 in the Y, so each layer has 36*39=1404 cells. If we divide 11126 by 1404, we get 7.9, which means this cell is in layer 8. We now go to layer 8 in the Grid Editor and see the cell with the Source/Sink in the upper left corner. IZoom in and right-click on the cell. Under Properties the cell ID is 11126, so this is the problem cell. Under Sources/Sinks we see that the user is injecting Water/Steam into this cell at a rate of 3.9 kg/s but with 0.0 enthalpy. BINGO! - zero enthalpy corresponds to water at absolute zero, so the cell is being cooled by very cold injection. We need to change the enthalpy to a realistic value. This means getting out the steam tables. You can either get out the old thermodynamics text or you can download an Excel spreadsheet from the Tools section of Help at our website at: http://www.thunderheadeng.com/petrasim.html.

Below is the steam table data for a temperature of 250 C and pressure of 2MPa (482 F and 290 psia). The enthalpy is 2901869.965 J/kg and the quality is pure vapor. So doing the calculation with this enthalpy would represent steam injection. Go to step 5.

```
Input Data Here                 English Units
Input (Do not change)
Temperature, C    250.00        Temperature, F  482.00
Pressure, Pa (abs)  2.00E+06    Pressure, psia  290.08
Quality, 0=L, 100=V             Quality, 0=L, 100=V 0
Spec volume, m3/kg              Spec volume, ft3/lb
Enthalpy, J/kg                  Enthalpy, btu/lb  0
Entropy, J/kg/C                 Entropy, btu/lb/f 0

Output                          Output
Temperature, C  250.00          Temperature, F  482.000
Pressure, Pa  2.00E+06          Pressure, psia  290.08
Quality, 0=L, 100=V 100.00      Quality, 0=L, 100=V 100.00
Spec volume, m3/kg  0.111450802 Spec volume, ft3/lb 1.7852
Enthalpy, J/kg  2901869.965     Enthalpy, btu/lb  1247.79
Entropy, J/kg/C 6544.287025     Entropy, btu/lb/f 1.5633
Tsat, C 212.38                  Tsat, F 414.3
Psat, Pa  3.98E+07              Psat, psia  576.90
Deg superheat, C  19.85         Deg superheat, F  67.7
Deg subcool, C  -17.78          Deg subcool, F  0.0
Viscosity, Pa-s 1.79E-05        Viscosity, lb-sec/ft2 3.74E-07
Crit velocity                   Crit velocity 1480.67
Density, kg/m3  8.972568916     Density, lb/ft3 0.5602
SG  0.009                       SG  0.009
Viscosity, poise (P)  1.79E-04
```

STEP 5: Change the enthalpy to an appropriate value, then try to run again. This might not fix everything. For example, maybe the rate you are using for injection will be larger than can be supported by flow to the adjacent cells and the pressure may become too large in the injection cell. This will again be an indication of an unrealistic problem.

Licensing/Registration Problems

On a few machines, a licensing error occurs when first running PetraSim. If you receive a message such as "NETWORK: Network drivers appears to not be serving this directory" or "INIT_NOT_SUCCEEDED", please perform the following steps:

1. Go to the installation directory C:\Program Files\PetraSim\
2. In this directory, double click (execute) the file SETUPEX.exe
3. You should now be able to run PetraSim and complete the registration process.

Contacting Technical Support

The PetraSim software is available for download at: http://www.thunderheadeng.com The same site provides PetraSim user manuals and example problems. Please follow the examples to become familiar with the software.

Questions and suggestions should be sent to support@thunderheadeng.com or by phone to +1.785.770.8511.

Mail should be sent to:

```
Thunderhead Engineering
1006 Poyntz Ave.
Manhattan, KS 66502-5459
USA
```

References

[Corey, 1954] A. Corey. *The Interrelation Between Gas and Oil Relative Permeabilities*. November, 1954. Producers Monthly. 38-41.

[Pruess, 2003] Karsten Pruess. *Personal communication*. 2003. email.

[van Genuchten, 1980] M. van Genuchten. *A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils*. 1980. Soil Sci. Soc.. 44. 892-898.

[Pruess, Oldenburg, and Moridis, 1999] Karsten Pruess, Curt Oldenburg, and George Moridis. *TOUGH2 User's Guide, Version 2.0*. November, 1999. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-43134.

[Pruess, 1992] Karsten Pruess. *Brief Guide to the MINC - Method for Modeling Flow and Transport in Fractured Media*. May, 1992. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBL-32195.

[Pruess, 1983] Karsten Pruess. *GMINC - A Mesh Generator for Flow Simulations in Fractured Reservoirs*. May, 1992. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBL-15227.

[Cengel and Boles, 1989] Yunus Cengel and Michael Boles. *Thermodynamics: An Engineering Approach*. 1989. McGraw-Hill, Inc.. 0-07-101356-9.

[Hirschfelder et al., 1954] J Hirschfelder, C. Curtis, and R. Bird. *Molecular Theory of Gases and Liquids*. 1954. John Wiley and Sons. New York NY USA .

[International Formulation Committee, 1987] International Formulation Committee. *A Formulation of the Thermodynamic Properties of Ordinary Water Substance*. 1987. IFC Secretariat. Dusseldorf Germany .

[Falta, Pruess, Finsterle, and Battistelli, 1995] Ronald Falta, Karsten Pruess, Stefan Finsterle, and Alfredo Battistelli. *T2VOC User's Guide*. March, 1995. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-36400.

[Pruess, Oldenburg, and Moridis, 1999] Karsten Pruess and Alfredo Battistelli. *TMVOC, A Numerical Simulator for Three-Phase Non-Isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated-Unsaturated Herogeneous Media*. April, 2002. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-49375.

[Xu, Sonnenthal, Spycher, and Pruess, 2004] Tianfu Xu, Eric Sonnenthal, Nicolas Spycher, and Karsten Pruess. *TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media*. September, 2004. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-55460.

[Moridis, Kowalsky, and Pruess, 2005] George Moridis, Michael Kowalsky, and Karsten Pruess.

TOUGH-Fx/HYDRATE v1.0 User's Manual: A Code for the Simulation of System Behavior in Hydrate-Bearing Geologic Media. February, 2005. Earth Sciences Division, Lawrence Berkeley National Laboratory. Berkeley CA USA . LBNL-3185.

[Versluys, 1931] J. Versluys. 1931. Bull. Amer. Ass. Petrol. Geol.. 15. 189.

[Barenblatt, et al., 1960] G. E. Barenblatt, I. P. Zheltov, and I. N. Kochina. *Basic Concepts in the Theory of Seepage of Homogeneous Liquids in Fractured Rocks*. 1960. J. Appl. Math. (USSR). 24 (5). 1286-1303.

[Scheidegger, 1957] Adrian Scheidegger. *The Physics of Flow Through Porous Media*. 1957. University of Toronto Press and Oxford University Press. London Great Britain .

[Edwards, 1972] A. L. Edwards. *TRUMP: A Computer Program for Transient and Steady State Temperature Distributions in Multidimensional Systems*. 1972. National Technical Information Service. Springfield VA USA .

[Narisham and Witherspoon, 1976] T. N. Narisham and P. A. Witherspoon. *An Integrated Finite Difference Method for Analyzing Fluid Flow in Porous Media*. 1976. Water Resour. Res.. 12. 57-64.

[Warren and Root, 1963] J. E. Warren and P. J. Root. *The Behavior of Naturally Fractured Reservoirs*. September, 1963. Society of Petroleum Engineers Journal. Transactions, AIME, 228. 245-255.

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